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Interface Design and Modelling, Wetting and High-Temperature Capillarity

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Abstract book

Federation of Materials Research Societies (FEMS) Swedish Society for Materials Technology (SFMT) Institute of Solid State Physics of the Russian Academy of Sciences (ISSP RAS) Grain boundary wetting by a second solid phase in the iron-based alloys

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Introduction/Purpose

A fundamentally new phenomenon has recently been discovered, namely the wetting phase transitions of the of grain boundaries (GBs) by layers of the second solid phase.

Methods

In this work we investigated the GB wetting transitions in the technologically important Fe-based alloys, namely the Fe-Nd-B-based hard magnetic alloys and Fe-Cr-based CROFER alloys used for the high-temperature applications like solid oxide fuel cells.

Results

The transition from incomplete to the complete wetting of grain boundaries by the liquid phase proceeds always with increasing temperature. It is because the temperature dependence of a GB energy in a solid phase intersects $\sigma_{GB}(T)$ with the temperature dependence of the energy of two solid/liquid interphase boundaries $2\sigma_{SL}(T)$. $2\sigma_{SL}$ always decreases with increasing temperatures stronger than the GB energy σ_{GB} since liquid phase has higher entropy in comparison with a solid one. In some cases the transition from incomplete to the complete GB wetting by a second solid phase also proceeds with increasing temperature like in Zn–AI and Fe–C systems. It is because GB energy in the α -phase $\sigma_{\alpha\alpha}$ becomes lower than the energy of two solid/ solid α/β interphase boundaries $2\sigma_{\alpha\beta}$.

Conclusions

If the wetting phase is also solid there is no simple reason, why $\sigma_{\alpha\alpha}(T)$ should decrease with increasing temperature stronger than $2\sigma_{\alpha\beta}(T)$. Indeed, we observed that the GBs can become completely wetted by a second solid phase with decreasing temperature. Moreover, the dependences $\sigma_{\alpha\alpha}(T)$ and $2\sigma_{\alpha\beta}(T)$ can intersect twice. In this case the GB dewetting transition would follow the GB wetting transition.

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Contribution of Academician Yu.V. Naidich into the field of high temperature capillarity

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Academician Yuriy Volodimirovich Naidich - outstanding internationally recognized Ukrainian scientist - has passed away. His contribution into the studies of capillary phenomena in metallic melts is well known. Academician Naidich pioneered many important topics of modern material science. He has proposed several approaches to control wettability of different types of materials by liquid metals: covalent ceramics, ionic crystals, and refractory metals. Diamonds, oxides, fluorides, carbides, borides, nitrides, perovskites are among them. More than 1500 contact systems were studied under the supervision of Yuriy Volodimirovich, many of them for a first time. On the basis of extensive experimental results Academician Naidich has formulated general principles of wettability by liquid metals based on the thermodynamic approach and recommendations for effective joining of materials of different nature. The most important of these principles are widely introduced in practice nowadays: addition of small amount of chemically active components to the substrate-inert melt in order to improve wettability (oxygen, sulfur, chlorine, complex anions) to improve wettability of ionic crystals by metallic melts. Many technological processes were developed under the supervision of Academician Naidich: metallization of diamond powder, refractory ceramic/metal joining for particles accelerators, nuclear reactors and spacecrafts, joining of ferroelectrics, sintering of super hard composites, etc.

Since 1964 Yuriy Volodimirovich was the head of The Department of Contact Phenomena and Nonmetal Materials Soldering of the Frantsevitch Institute for Problems of Materials Science of NASU. He authored more than 800 articles and patents, and 12 books. He was the Chief Editor of «Adhesion of melts and brazing of materials» published since 1976. Academician Naidich has educated 40 PhDs and Doctors of Science, gave lectures at Physics Department of Taras Shevchenko National University of Kiev. He have organized over 10 scientific conferences in USSR and Ukraine, and he was among the founders of international "High Temperature Capillarity" conference, which is held regularly all over the world since 1994.

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Interfacial reactivity in liquid Ni alloys-oxides systems: experiments and modelling

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Introduction/Purpose

Investment casting processes of Ni-based superalloys involve the contact between molten alloys and the ceramic materials that are used as cores or shells. For this reason, information about the high temperature interactions between liquid alloys and refractory oxide materials is of practical importance in order to select the most proper metal-ceramic combinations and processing parameters.

Methods

Such information may be obtained experimentally from specific wetting tests with improved procedures followed by microstructural and microchemical characterization. At the same time, the thermodynamic modeling by CALPHAD of the reactivity in alloys-oxides systems allows to interpret the experimental findings, to foresee the interfacial reactivity and to perform extrapolations toward non-studied domains of temperature or composition. In this talk, these topics will be covered with reference to the project INSURFCAST (INnovative SURFaces for superalloys CASTing processes). The wetting behavior of Ni alloys in contact with oxides chosen among those used or that can be potentially used for melting and casting of superalloys (e.g. Al₂O₃, ZrO₂, ZrSiO₄, Kaolin)) will be presented. Alloys include both simple Ni alloys containing small additions of reactive solutes (e.g. Al, Hf, Cr) and commercial alloys (e.g. CMSX4, Hayness 282®)).

Results

Wetting tests by the sessile drop method and characterization by SEM, EDS, confocal profilometry, XRD, etc. demonstrated the role of reactive elements in the formation of new oxides in the form of layers or inclusions that may affect the quality of the final product. Results were also interpreted by the determination of the relevant thermodynamic data (phase diagrams, activities, energy quantities) obtained by CALPHAD.

Conclusions

These results can have an importance that goes beyond the casting industry, as they can be helpful in the design of advanced metal-ceramic brazing processes, production of Metal-Matrix-Composites as well as of coatings for high temperature applications.

Acknowledgements

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Large scale kinetic Monte-Carlo modeling of grain growth in tungsten

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Introduction/Purpose

Tungsten is a material considered for first wall material in Tokamaks. At elevated temperatures, it is susceptible to recrystallization which makes it brittle and prone to mechanical failure. An increased recrystallization temperature could allow higher operating temperatures and thus higher thermodynamic efficiency. This makes recrystallization temperature an important parameter in fusion materials design, and its prediction an important modeling challenge. The recrystallization phenomenon is driven by nanoscale defects and how they influence the evolution of micron-scale grains, making it inherently multi-scale and hard to address with current simulation techniques.

Methods

We have developed a parallel kinetic Monte-Carlo (KMC) code, SPOCK, with which we can reach large enough length- and time-scales to study grain boundary motion and grain growth in polycrystalline materials, while retaining atomic scale resolution. The SPOCK code is to our knowledge the only exact parallel KMC code, which means that it can simulate systems with micron-scale grains, without suffering from artefacts due to domain decomposition and parallelization approximations like many other KMC codes do. With SPOCK we have performed the largest grain growth simulations to date, and efficiently employed 400,000 processor cores.

Results

We are currently developing grain boundary models for W as a first wall material. Using molecular dynamics we extract relevant parameters for motion of grain boundaries and their interaction with other defects. We will present results on large scale molecular dynamics simulations of W grain boundaries and grain boundary migration, as well as micron scale KMC simulations of growth in polycrystalline W containing hundreds of grains. Acknowledgement: This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.



Modelling of grain boundary complexions stability in Ni/Bi system

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Introduction/Purpose

The concept of controlling the properties of polycrystalline materials through a directional change of grain boundaries (GB) properties, so-called GB engineering, is actively developed. Segregation of the active component in multicomponent metallic systems can improve the characteristics of materials, but it is also able to cause embrittlement of polycrystals, which leads to catastrophic consequences. However, there is no universal approach, which allows predicting the stability of GB complexions for an arbitrary GB.

Methods

We present a holistic approach that allows predicting the stability of the arbitrary GB complexion using a predictive model — an artificial neural network. As a training dataset, the results of DFT simulations obtained for a set of preselected atomic configurations were used. We explore as a model Ni/Bi system that is of significant practical importance [1]. Energy values were obtained for a set of both high-symmetric and general GBs using the trained neural network. "Clean" GBs, as well as configurations containing Bi mono- and bilayers were studied.

Results

The proposed approach provided an insight into the stability regions of GB complexions in five-dimensional space, which is used to describe the structure of a GB. The results of our model for distinct GBs are consistent with previously obtained experimental data [1].

The Brandon criterion, which was previously applied to distinguish between special and general GBs, has also been revised. The reported study was supported by RFBR under the research project № 18-33-00842

Conclusions

Neural networks were found to be an effective tool for GB energy and composition prediction

Acknowledgements

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Non-reactive wetting of metals by liquid Ag

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Introduction/Purpose

Wettability in multicomponent metallic systems is widely studied due to practical and fundamental importance. The last is connected to the possibility of linking interfacial energies of appearing interfaces by means of famous Young equation. Interfacial thermodynamics is determined by interatomic interaction and tightly linked to bulk thermodynamics of corresponding phases, but this link is not revealed to the moment. One of the key factors, which complicates quantitative analysis of interfacial thermodynamics on the basis of Young equation is the formation of wetting precursors in front of the triple line. Such atomically thin films (called "complexions" in modern literature) decreases significantly (in some cases more than twice) the surface energy of solid metals. The purpose of the present study was to analyze wettability and interfacial thermodynamics in Ag/X systems, where X are the metals with different affinity to silver

Methods

Polycrystalline Cu, Ni, Nb, Co, Mo, W were selected as substrates, as they do not form intermetallics with Ag, but demonstrates different solubility in liquid silver-based alloys. Experiments were performed in reductive atmosphere slightly above silver melting temperature by means of dispensed drop modification of classical sessile drop technique. Images of spreading drop were recorded with high-speed video camera with 1000 fps. Surface of substrates was analyzed with XPS in order to detect precursor film

Results

Contact angle of silver on studied substrates growth from values close to zero observed for copper substrates to about 50 deg in the case of W. Such growth of contact angle correlates with growth of heat of mixing at infinite dilution for corresponding metallic couple. We have observed similar behavior for the number of Pb/X systems, were X are different metallic substrates.

Conclusions

Correlation of wettability with heat of mixing at infinite dilution seems to be a general trend for non-reactive metallic couples

Acknowledgements

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Phase-field modeling for simulation of immiscible multiphase flows and its application to metallic foams

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Introduction/Purpose

A new model based on the phase-field method is developed for simulation of immiscible multiphase flows.

Methods

Each phase, α , is characterized by one phase-field parameter, φ_{α} , and the corresponding density is defined as a function of φ_{α} and the total mass of phase α . To account for the interface induced force in the fluid dynamics of multiphase flow, an interfacial force is added to the right hand side of Navier-Stokes equations. On the other hand, the non-conserved phase-field equation is coupled to the Navier-Stokes equations to account for the effect of flow on the interface dynamics.

Results

The model is validated for the case of static equilibrium of a 2D bubble (Young-Laplace law) for different values of the interface energy. Moreover, the expected effect of interface energy on the dynamics of two coalescing bubbles is born out. Finally, the model is applied to study microstructure evolution in metallic foams.

Conclusions

A specific feature of this model is that the interface and bulk free energy contributions to the interface dynamics are separated. This characteristic of the present model allows to tune the rate of coalescence compared to other concurrent processes. Therefore, it facilitates the use of model to study physical problems concerning interfacial dynamics of bubbles in the presence of flow and their coalescence in the microstructure evolution.

Some Factors Controlling Pressure Solution Rate

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Introduction/Purpose

Pressure solution (PS) is a fluid-assisted process driven by the excessive stress-induced chemical potential of solids. It is intensively studied as a mechanism responsible for the rocks deformation in the crust, for deterioration of monuments, as a mechanism of liquid sintering etc The mass transfer is achieved through material dissolution at stressed sites, diffusion and re-precipitation. In this study, we discuss possibilities of controlling the overall process rate.

Methods

PS creep rate has been assessed on calcite and NaCl samples submitted to powder compaction or ball indentation in contact with aqueous solutions.

Results

The cyclic loading was shown [1] to accelerate dramatically the creep of several materials (e.g. NaCl powder) known to pass into solution in the diffusion-limited regime. In this study, we have tested NaCl in the presence of increasing amounts of urea (which is well known to have an adsorption affinity for the salt surface). Urea additives reduced the sensitivity of NaCl to cyclic loads, which indicates to a the shift of kinetics towards interface-limited. In order to assess the effect of adsorbing species present in the liquid phase on the PS creep rate, we have studied the behaviour of calcite in the presence of typical anionic (sodium dodecyl sulfate) and cationic (cetylpyridinium chloride) surfactants over a wide concentration range (the impact of chimisorbed chelating compounds strongly interacting with CaCO3 surface was reported earlier [2]). The adsorption energy for surfactants studied is considerably lower; nevertheless even a reversible Langmuir-type adsorption of surfactants reduces noticeably the PS rate of calcite. The values for surface coverage found from the creep deceleration and from independently measured adsorption and zeta-potential practically superpose, which confirms that the effects observed are adsorption-induced.

Conclusions

The pressure solution of calcite and rock salt may be controlled by applying physical (cyclic loading) or chemical (adsorbing additives).

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Structures and transitions in bcc tungsten grain boundaries

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Introduction/Purpose

Grain boundaries greatly influence many properties of engineering materials. Accurate prediction of their structure and possible transitions using atomistic modeling are important for strategies that aim to improve properties of materials. While grain boundaries created by the γ - surface method as a union of two perfect half crystals have been studied extensively, it is known that the method has limitations and does not always predict the correct ground states.

Methods

In this work, we use a newly developed computational tool, based on the USPEX structure prediction code, to perform a grand-canonical search of grain boundaries in bcc metals.

Results

We find new ground states and multiple phases that cannot be described using the conventional structural unit model. The new ground states are confirmed by first-principles calculations. We use molecular dynamics simulations to investigate high- temperature structures of these boundaries and transitions induced by absorption of point defects.

Conclusions

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.



Study of Effect of Composition of Steel and Holding Time on the Microstructure Evolution in Steel/Cu/Steel Joints.

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Introduction/Purpose

Various steels are being used in the industries for different structural applications and the joints required are fabricated using copper and its alloys as the joining material. However well performing these joints are for the industry, their efficiency and reliability are still a drawback. Various research studies have been taken up to understand why this happens and the problem has been defined from thermodynamic point of view. The current study undertaken tries to answer the problem from the compositional point of view of the steels.

Methods

The method of experimentation employed is as andwich system where copper foil is sandwiched between the steels and the experiment was conducted in an inert gas environment. at holding temperature of 1100°C. The experiment was conducted at different holding times to study the effect on the observed microstructure.

Results

The structural steels have different alloying elements like Cr, Mn and S which are known to form intermetallic compounds which have a fatal effect on the joint thus formed. In our study we found the diffusion of Cr, Mn and S from the bulk of steel to the joint interface and precipitation of these elements into compounds like MnS, (Cr-Cu-Mn-S) complex compound at the experimental temperature. These precipitates served as sites for crack initiation which causes the failure of the joint. The cracks arise from the volumetric expansion mismatch between these compounds and the molten copper layer upon cooling. The diffusion of these elements increased as holding time is increased.

Conclusions

In conclusion, the diffusion of elements like Cr, Mn, S from bulk of the steel to the molten copper at the applied temperature and time was calculated and their effect on the subsequent joint microstructure was studeid. The study also aimed at drawing an optimum time after which the formation of the aforementioned compounds was observed.

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Wettability Changing Effects of High-Energy Surface Treatments

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Introduction/Purpose

One of the biggest development discipline todays is the automotive weight reduction. The manufacturers are focusing on making new hybrid materials pairing and innovative technologies that satisfy the newest requirements. One of them is the hybrid materials pairing in the different part of the body, like aluminum-glass fiber and carbon fiber reinforced composites or new type of high strength steels. These joining technologies have to complete the newest requirements.

Over the last decade, the number of researches has increased in the field of bonding technologies. Researchers attempt to improve surface adhesion properties by surface modifications. Adhesion bondings like adhesive and soldering is two of those bonding techniques, where it is important to analyse the preparation of the surfaces. One such surface property is wettability, which can be improved by several types of surface treatment.

Methods

In this research the main focus was to modify the surface of the different metal substrates without any damaging on the topography. In recent years, atmospheric pressure plasmas and femtosecond impulse lasers have appeared, with which research is ongoing on surface treatments. Two type of innovative surface treatments were examined. The effects of plasma surface treatment at atmospheric pressure and femtosecond impulse laser surface scanning were investigated.

Results

When the surfaces change to hydrophilic because of the high energy activation, adhesion binding technologies were performed. In order to find out the process of the activation on the surface, wettability was determined. The strength of the overlapped joints were increased significantly. The topography of the materials were analysed, to establish the physical connection between the wettability changing and the increased strength of the connections.

Conclusions

The high-energy treatment could change the surface wettability to hydrophilic, while the strength of the adhesion joint could be multiplied. In addition, we summarized the theoretical background of adhesion, surface tension and surface treatments.

Wetting and interfacial behavior of Si-ion implanted SiC substrate by molten pure AI, Cu and Sn

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Introduction/Purpose

Silicon carbide (SiC) is one of the most widely applied semiconductor materials. The wetting of metal/SiC system plays a crucial role in the fabrication of the SiC-reinforced metal-matrix composites, brazing of SiC ceramics and packaging of SiC semiconductor devices. High dose and/or high energy of ion implantation into SiC monocrystal substrate can cause high concentration of defects (lattice damage or disorder and vacancies), which can affect the wettability of molten metals on the SiC monocrystal substrate.

Methods

Three doses (5×10¹⁵, 1×10¹⁶ and 5×10¹⁶ ions/cm²) of Si ion were implanted into C-terminated and Si-terminated SiC monocrystal substrates with an energy of 20 KeV at room temperature. The wetting of Si-implanted SiC (Si-SiC) by molten pure AI, Cu and Sn was investigated using the sessile drop technique in a high vacuum (4×10⁻⁴ Pa) at 1323, 1373 and 1273 K, respectively. The surface characteristics and interfacial behavior of metal/Si-SiC systems were analyzed and discussed.

Results

The experimental results showed that the equilibrium contact angles of Al/Si-SiC and Cu/Si-SiC systems were increased more or less with the Si implantation dose increasing. The contact angles of Al and Cu on C-terminated Si-SiC were lower than those on Si-terminated Si-SiC while employing the same Si implantation doses, respectively. Moreover, the contact angle of Sn on C-terminated Si-SiC decreased significantly from 155° to 60°, while that of Sn on Si-terminated Si-SiC kept at ~125°.

Conclusions

These phenomena indicated that the wettability of metal/ion-implanted SiC systems can be closely related to the reactivity between metal and SiC and to surface polarity of SiC substrate.

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Wetting and interfacial reactivity of liquid zinc-aluminium on pure iron and FeAl alloys after recrystallization annealing.

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Introduction/Purpose

The understanding of gas-metal reactions and subsequent surface wettability at high temperatures is often limited due to the lack of in-situ surface characterization.

Methods

Within this objective the High Temperature Wettability Device (HTWD) was designed to allow the in-situ characterization by X-rays Photoelectron Spectroscopy (XPS) of the sample surface after annealing and the deposition of a liquid metal droplet for wettability measurements. The heat treatment is performed in an infra-red lamp furnace in a well-controlled atmosphere designed to reproduce gas-metal reactions occurring during the industrial recrystallization of steels. The in-situ characterization gives access to the real composition of annealed surfaces without any contamination by ambient atmosphere. The wetting experiments are carried out by dispensed drop technique with the precise control of the droplets kinetic energies. The spreading of drops is recorded by high speed CCD video-camera at 500-1000 frames/s to get information at very low contact time.

Results

Experiments of zinc-aluminium drop deposition on pure iron samples are performed to serve as references for further experiments on other substrates. They allow to control with XPS the deoxidation of iron during annealing and to study the influence of substrate and drop temperatures on the wetting behaviour. FeAI alloys were studied to simulate different surface chemistries and morphologies that can be obtained during recrystallization annealing at different atmosphere dew points. The wetting of the annealed surfaces with zinc-aluminium is conducted to understand the incidence of the annealing conditions on the reactive wetting of these steel grades during hot-dip galvanizing.

Conclusions

Wettability change on the studied samples is explained by the modification of the surface chemistry depending on the recrystallization annealing conditions.

Wetting and reactivity of carbon by Ag-Cu-In-Ti and Sn-Ag-Cu-Cr alloys for brazing applications

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Introduction/Purpose

Brazing of carbon by liquid alloys at low temperatures is a challenging issue. In this context, the wetting and reactivity between Ag-Cu-In-Ti (melting point: $500 - 600^{\circ}$ C) and Sn-Ag-Cu-Cr (melting point ~ 323° C) active alloys with different carbon substrates have been studied.

Methods

Experiments were carried out between 720°C and 920°C under high vacuum (10⁻⁴ Pa) using the sessile drop method and the spreading kinetics were determined by image capture system using a CCD camera.

Results

Very low final contact angles were obtained with Ag-Cu-In-Ti at temperatures above 770°C, but no wetting was reached below this temperature. The spreading kinetics of the wetting process strongly depends on the experimental temperature and the type of the carbon substrate (vitreous, pyrolytic or graphite) and it was found to be controlled by the local reaction kinetics at the triple line. Low final contact angles were observed with Sn-Ag-Cu-Cr alloy on vitreous carbon at 720-900°C. However, a drastic increase in the spreading kinetics was observed between 800 and 900°C for this alloy.

The morphology and the composition of the reaction layers formed at the reactive alloy/substrate interfaces were characterized by SEM, TEM and EDX. At the Ag-Cu-In-Ti/carbon interface, a reaction layer some micrometer thick was found to be formed. This layer grows in a columnar way and its thickness increases from the triple line to the center of the drop as well as with the holding time. Moreover, a very thin TiC_x reaction layer was also observed between the carbon substrate and the columnar layer. At the Sn-Ag-Cu-Cr/carbon interface, a reaction layer some micrometer thick was found to be formed and it seems to correspond to Cr_3C_2 compound (further analysis are in progress to confirm this result).

Conclusions

Finally, some examples of brazing of carbon by these alloys will be presented.

Introduction/Purpose

It is important to know wetting and spreading phenomena between slags and refractories. This knowledge provides a better understanding of inclusion removal and of penetration behavior of slags [1, 2]. Although the values of surface tension and viscosity of slag can be easily found, the contact angles cannot be obtained in open literatures due to difficulty of the measurement. Recently, the dispensed drop technic with a high speed camera provided intrinsic values both of wetting angle and spreading rate for the system between slags and reftractories such as Al₂O₃, MgO, MgAl₂O₄ [3~5] In this presentation, recent experimental data between CaO-SiO₂ slags and SiO₂ will be shown and disscussed based on the slag chemistry.

Methods

The slag and substrate are separately heated at 1600°C and the molten liquid droplet of slag is dropped onto the substrate by the push bar, so the droplet is contacted with the substrate in isothermal condition (Fig.1). A high speed camera (1000 frame/sec) is used to capture the images of the whole process of wetting. After the experiment, the cooled samples are analyzed by SEM and EDS.

Results

The contact angle and the spreading rate have determined by changing slag chemistry of CaO-SiO₂ slag; One is SiO₂ saturated and the other is non-saturated at 1600°C.

Since the slags have different physical properties such as viscosity, surfac tension and density etc, the wetting and spreading behaviors are different. Especially, viscosity of the slag significantly changed the contact angle and spreading rate. Lower viscosity provided much faster spareding rate and lower wetting angle. The reaction between lquid slag and solid substarte also provided lower wetting and faster spreading.

Conclusions

- 1) The low viscosity of CaO-SiO₂ slag provided much faster spareding rate and lower wetting angle.
- 2) The reaction between lquid slag and solid substarte also provided lower wetting and faster spreading.

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Fig.1 – Dispensed drop apparatus with a high speed camera.

Wetting Properties of Surface Treated Automotive Polymers

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Introduction/Purpose

As a result of stricter environmental and safety standards, vehicle manufacturers have to reduce the weight of the vehicles, because 10% weight loss cause 8-10% reduction of fuel consumption. To reduce the weight and increase safety, vehicle manufacturers use new polymer pairings. These materials has a needed in different industry sectors to improve the performance of polymer surfaces for different joining technologies, which cannot be fulfilled by the conventional surface modifications and coatings. Surface engineering is rapidly developing because of the presence of new and more cost-effective methodes. The compact and energy efficient atmospheric pressure plasma and femtosecond impulse lasers have higher process efficiency, making them more attractive for integration into a manufacturing line.

Methods

This research goal is to change the surface energy of different materials such as polymers without modificating the surface topography. The wetting angle was measured on the surface layer after the different high energy surface treatments.

Results

Better understanding of high energy surface activation requires explanation of the relation between the basic mechanisms of high energy treatments. For this the wettability changing effect of the surface modification methodes were investigated using contact angle measurement. The macro geometry of the activated connecting materials, the tension stress of the bonded pairing and the breaking method were investigated during the reseach.

Conclusions

The treated surfaces change to hydrophilic because of the high energy activation. The contact angle is significantly reduced as a result of the treatment. The strength of the examined joints were significantly improved.

Bulk and grain boundary phase transformations in Al-10 wt.% Mg alloys during high pressure torsion

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Introduction/Purpose

In recent years attention has been paid to studies of the structures and properties of ultrafine-grained metals and alloys using various methods of severe plastic deformation. It is known that severe plastic deformation, in particular, the high-pressure torsion (HPT) can greatly change the structure of the material, lead to the formation of metastable phases not only in two-phase region of the phase diagrams, but also in a single-phase region.

Methods

The goal of this work is to study the microstructure of Al–10 wt.% Mg alloy after HPT-treatment in a two- and singlephases regions of the phase diagram due to heated in a differential scanning calorimeter (DSC) from 25 to 500 °C.

Results

DSC data showed that DSC curve has pronounced peaks: one endothermic peak at the temperature of 106 °C and three exothermic peaks at temperatures of 182 °C, 258 °C and 315 °C. And also small peaks near the temperature of 400 °C. The structure of the alloy was investigated at these temperatures.

Conclusions

Data of transmission electron microscopy and X-ray analysis showed that with an increase in temperature in the Al– 10 wt.% Mg alloy after HPT-treatment the solid solution decomposes without the phase diagram, but with the formation of metastable phases: GP zone $\rightarrow \beta \rightarrow \epsilon \rightarrow \beta \rightarrow \gamma \rightarrow \beta$. Comprehensive analysis of Grain Boundary Character Distribution — Grain Boundary Energy Distribution relationship for FCC metals

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Introduction/Purpose

Due to the absence of reliable experimental data and the complexity of description, a function that could describe the structure-property relationship for the whole variety of grain boundaries in FCC metals is still not available. During last decades most of works analyzing GBCD–GBED relationship on big datasets deals with the determination of dihedral angles in triple junctions treated in the framework of capillary vector approach [1]. This method is based on the assumption that the whole space of GB structural parameters can be divided into equal size domains with constant energy, which could not be the case near GBs with special properties.

Methods

In this study, more "traditional" approach is explored — the energy of around 500 GBs in copper polycrystalline foil was determined from dihedral angles formed in the vicinity of GB grooves assuming isotropy of solid/gas surface energy. Dihedral angles and GB traces orientations were measured from 3d reconstruction of the foil surface obtained with optical interferometer.

Results

In agreement with previous findings [2] it was demonstrated, that only part of $\Sigma 3$, $\Sigma 9$, $\Sigma 17 \mu \Sigma 33$ GBs have demonstrated decline of the energy. Reverse dependence of GB population and energy was detected only for $\Sigma 3$ boundaries: decrease of total GB energy due to preferential orientation of GB planes perpendicular to the sample surface dominates.

Conclusions

It was also demonstrated that GBs with both low index planes including {100}/{100}, {111/111} and {110}/{110} possess significantly lower energy.

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Grain boundary wetting in W-Ni alloys

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Introduction/Purpose

Wetting phenomena play an important role in the manufacturing of products from heavy metals like W, Mo etc. In the current study the wetting grain boundary phase transitions were investigated in W–Ni system.

Methods

W–Ni alloys of various compositions were prepared by sintering followed by the heat treatment at different temperature. Structure of the obtained alloys was investigated by means of transmission electron microscopy.

Results

Grain-boundary wetting phase transitions in the W-Ni binary system were investigated. Grain boundaries with different types of the grain boundary complexions were detected in the alloys annealed in single-phase area of the phase diagram:

- 1. grain boundaries with incomplete or partial wetting: particles of the wetting phase are in either triple joints or as lenticular inclusions along the boundary line; the contact angle is nonzero; the wetting phase is absent at the interface between two grains;
- 2. grain boundaries with complete wetting: the wetting phase forms a layer of variable thickness along the interface and the contact angle at the triple junction is zero;
- 3. grain boundaries with pseudo-partial wetting: observed when the contact angle in the triple junction is nonzero, but a thin (~ 5 nm) wetting layer is present along the interface wetting phase.

A nickel-rich phase was found at the grain boundaries in the alloys annealed in the single-phase area. This is the socalled grain-boundary phase, which is unstable in the sample's bulk and can exist only at the grain boundary.

Conclusions

The obtained structural data were used to construct the lines of grain boundary wetting and pre-wetting phase transitions on the W-Ni bulk phase diagram.

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Highly thermally conductive graphene fibers

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Introduction/Purpose

New fibers with excellent and rich functionalities have been untiringly pursued by researchers. Graphene is a known material with excellent conductor of electricity and heat. Therefore, the graphene fiber has gotten a lot of attention. The development of an effective strategy for fabrication is vital for graphene fiber.

Methods

Because graphene isn't meltable, it is impossible to assemble graphene into fibers by the melt spinning processes. The graphene fiber is produced by upon reduction of the GO fibers, while graphene oxide (GO) fibers can be assembled from a dispersion of GO in aqueous media. High enough concentrations of GO are needed for efficient alignment and effective coagulation. Hence, we enhance the degree of dispersity of GO by adjustment of PH value through dilute hydrochloric acid and ammonia. Then the GO fiber is fabricated by loading the GO dispersion agent into an injector and injecting the agent into a coagulation of a 5 wt% CaCl₂ soultion. The Ca²⁺ ionic cross-linking between graphene sheets could further enhance mechanical strength of GO fiber. GO fiber is collected and is reduced into graphene fiber by hydroiodic acid.

Results

A graphene fiber with high thermal conductivity has been obtained. The conductivity of the graphene fiber 200 Wm⁻¹K⁻¹

Conclusions

We believe more graphene macrostructures with remarkable properties for many promising applications will be fabricated by wet spinning. And other 2D sheets may also be assembled into macrostructures by wet spinning.

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High Temperature-Reactivity evaluation of AI-Ti alloys in contact with SiC

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Introduction/Purpose

Several industrial processes interested in coupling SiC to AI-Ti alloys (e.g. metallization of SiC components, brazing of SiC parts) require a deep knowledge about AI-Ti/SiC interactions occurring at high temperatures.

Methods

To this end, the surface reactivity between SiC and Al-Ti alloys (Al₃Ti and (Al+Al₃Ti) systems) has been analyzed by specific experiments (wetting, DSC, microstructural examinations) as well as by a thermodynamic approach (CALPHAD method).

Results

An Al-C-Si-Ti thermodynamic database has been successfully set up to calculate several sections and projections on which a comparison was made possible of the computed, expected solid phases formed at interface with the ones characterized in wetting experiments. By this means, the evolution of liquid and solid phases has been interpreted and discussed, defining the $Ti_3(Al,Si)C_2$ mixed MAX-phase as the main interfacial product coming from the chemical reaction, as a function of temperature and alloy composition.

Conclusions

This work provides a guide for the choice of the operating parameters in processes such as brazing or SiC metallization in microelectronic applications, in which the control of the interfacial products is one of the most delicate production step. The proposed approach to follow the pathway of liquid composition with time and temperature during liquid/solid interaction, successfully applied to interpret the microstructure obtained in wetting experiments, is a promising way to interpret more complex cases such as homogeneous or even heterogeneous brazing processes.

Influence of annealing duration on the wetting structure formation

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Introduction/Purpose

The investigation of the wetting phase transition is an interesting topic in modern material science. It is important not only for industrial application, such as welding, soldering or structure formation at elevated temperatures but also as fundamental grain boundary effect. The investigation of wetting in polycrystalline systems is the best way to investigate both model and real alloys, but it has some drawbacks. In particular, the recrystallization and grain growth rate if the wetting phase is liquid. The goal of this work was to show the influence of these factors on the wetting structures after different heat treatment.

Methods

A set of samples of two alloys (Mg cast alloy EZ33A and Cu – Ag) was annealed with different durations at elevated temperatures where the liquid phase grain boundary wetting occurs. The chosen durations were 0.5h, 2h, 5h and 62h. After annealing the samples were quenched in water. The microstructure of the samples was analyzed by scanning elector microscopy and electron backscattering diffraction.

Results

The investigation shows the influence of the grain growth and recrystallization on the formation of wetting structures in the liquid phase grain boundary wetting regime. The recrystallization of all samples was finished in the first 30 min. After that, the samples had already much bigger grain size than in the initial state. The following grain growth is much slower than the grain growth at recrystallization.

Conclusions

In grain boundary wetting investigation on polycrystalline samples, it is important to anneal the alloys long enough for the recrystallization to end. After that, the grain growth changes the sample structure too slowly and insignificantly. As the most liquid metal wetting happens either at soldering or welding or at the destruction of parts at high temperatures the long-time changes in the wetting structures are less important than the stabilization of the structure after recrystallization.

Selected references

The investigation of the Cu – Ag system was performed with the financial support of the Russian Foundation for Basic Research (Project # 18-33-00473).

The investigation of the EZ33A alloy was performed with the financial support of the Russian Science Foundation (Project # 18-72-00243).

Influence of cooling rate on the wetting structure formation.

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Introduction/Purpose

The investigation of the wetting phase transition is an interesting topic in modern material science. It is important not only for industrial application, such as welding, soldering or structure formation at elevated temperatures but also as fundamental grain boundary effect. The investigation of wetting in polycrystalline systems has some drawbacks. In particular, insufficient cooling rates at quenching lead to reversed wetting and growth of the nearby grains into the liquid. That can deform the grain boundary shape and for false contact angles. The goal of this work was to show the influence of these factors on the wetting structures after different types of quenching.

Methods

A set of samples of two alloys (Mg cast alloy EZ33A and Cu – Ag) was annealed for 2h at elevated temperatures where the liquid phase grain boundary wetting occurred and cooled or quenched in different ways. The microstructure of the samples was analyzed by scanning elector microscopy and electron backscattering diffraction.

Results

The investigation shows the influence of different cooling rates on the fixation of the liquid phase grain boundary wetting structures. It was shown that at insufficient cooling rates the wetting structure changes very fast. The grains grow into the liquid, close the liquid canals between triple junctions and reconstruct the melted grain boundary. Sometimes, the grains grow dendrite-like shapes that make the grain boundary into a wave. The contact angles formed on the grain boundaries do not represent the real energy equilibrium at the given temperature.

Conclusions

In grain boundary wetting investigation on polycrystalline samples, it is important to choose the quenching method that will be used for a specific experiment. At moderate annealing temperatures the quenching in water is fast enough, but at higher temperatures quenching in liquid nitrogen, with the destruction of the ampule under the nitrogen surface, is required.

Selected references

The investigation of the Cu – Ag system was performed with the financial support of the Russian Foundation for Basic Research (Project # 18-33-00473).

The investigation of the EZ33A alloy was performed with the financial support of the Russian Science Foundation (Project # 18-72-00243).

Influence of faceting grain boundary phase transition on wetting of grain boundaries

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Introduction/Purpose

The equilibrium contact angle at wetting phenomena is determined thermodynamically from the condition of minimality of free grain boundary (GB) energy and must have a single value. However, experimental studies show that the measured contact angles often take different values. The reason is phase transitions of faceting on the GB. This work is devoted to the manifestation of phase transitions of faceting at GB at wetting.

Methods

Two-dimensional bicrystals with a tilt [11-20]GB with 35° , 57° and 85° disorientation angles and bicrystals with a tilt [10-10] GB with $30^{\circ} \div 53^{\circ}$ disorientation angles were grown from high-purity Zn (99.999 wt.%) using the modified Bridgman method. The temperature of the phase transition of faceting (appearance and disappearance of the GB facet) was determined in-situ during isothermal annealing by changing the shape of the moving boundary, the disappearance of the facet.

Results

The results of an experimental study of the movement of individual tilt GBs in the form of a half-loop in zinc, the determination of the temperature of the phase transition of faceting (the appearance-disappearance of facets at moving GB) are presented. Theorists suggest that the disappearance of facets at GB as internal interfaces should occur above 0.7 T of melting. The figure shows the microstructure Ti-10%Nb, illustrating the different degree of wetting of GBs at an isothermal annealing temperature 800C during 912h. On the GB 2 wetting is not observed, perhaps because the temperature of the phase transition above the temperature of isothermal annealing. On GB 1 the observed wetting is likely that the phase transition temperature is of below the temperature of isothermal annealing.

Conclusions

To obtain a structure with isotropic properties it is necessary to choose the temperature of isothermal annealing for wetting above the temperature of the faceting GBs.



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Influence of HPT and pre-annealing on the microstructure and hardness of Ti - V and Ti - V - AI alloys

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Introduction/Purpose

The severe plastic deformation strongly changes the microstructure and properties of titanium-based alloys.

Methods

The structure and microhardness of four binary and ternary titanium-based alloys (Ti–4 wt.% V, Ti–4 wt.% V–6 wt.% Al, Ti–4 wt.% V–3 wt.% Al, and Ti–5 wt.% V–6 wt.% Al) have been studied after preliminary annealing and following high pressure torsion (HPT).

Results

After HPT, the Ti–4 wt.% V alloy contains much less (ω Ti) phase than Ti–4 wt.% Fe and Ti–4 wt.% Co alloys [1]. The addition of aluminum to the binary Ti–V alloys completely suppresses the formation of the high-pressure (ω Ti)-phase. HPT leads to the partial decomposition of the annealed (α Ti) solid solution and "purification" of α -phase similar to that in the Ti–Fe alloys.

FIG. Bright-field TEM micrographs for (a) Ti–4 wt. % V and (b) Ti–4 wt. % V–6 wt. % Al alloys after annealing at 700 °C and after HPT. The insets in (a) and (b) show selected area electron diffraction patterns. (c) and (d) Radial intensity distributions respective to the diffraction patterns in (a) and (b). Intensities were integrated along the Debye rings. Blue bar charts show the positions of the reflections from (α Ti). Green bar charts show the positions of the reflectional peaks from one of the titanium aluminides with tetragonal lattice, most probably Ti2Fe.

Conclusions

After HPT of the studied ternary alloys, the (β Ti)-phase completely disappears and nanoparticles of Ti2Fe form instead. This fact explains why the addition of aluminum leads to the increase of microhardness of alloys after annealing between 600 °C and 950 °C and after HPT-treatment. The increase of the temperature of the preliminary annealing also increases the hardness of all alloys after HPT-treatment.

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Influence of kinetic grain boundary properties on wetting of grain boundaries Vera Sursaeva¹, Alena Gornakova¹, Alexander Straumal¹

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Introduction/Purpose

The phenomenon of wetting at the grain boundaries (GB) has a thermodynamic point of view and a kinetic aspect. In the process of isothermal annealing there are two parallel processes: grain growth and wetting, that is, the movement of GBs and triple junctions with the particles of the second phase. The particles dragging of the second phase is comparable with triple junctions dragging when the particle size is 10⁻⁵ m. The grain growth is slowed not only by the triple junctions and second-phase particles but also defects on the GBs. The presence of such GB defects on GB as GB edges and GB facets should contribute to the partial wetting of GBs, which is observed in the figure (Ti-20%Nb, 600C, 786h, section 2 and 3).

Methods

The shape and displacement of the moving GB was studied in the temperature range 220÷401C in situ in a high-temperature attachment to an optical microscope using polarized light

Results

The paper presents the results of an experimental study of the movement of individual tilt GBs in the form of a halfloop in zinc with GB defects as facets and GB edges. Under the study of kinetic properties, we mean the experimental determination of the mobility of GBs, parameters of the motion dragging of GBs with the facets and edges. Two-dimensional bicrystals with the tilt GB with orientation angles of 35°, 57° and 85° and the bicrystals with the tilt GB and angles of orientation of 30° ÷ 53° were grown from high-purity Zn 99.999 wt.%, using the modified Bridgman method.

Conclusions

It is found that the presence of a GB edge at GB reduces the mobility of GB system by an order of magnitude. It is demonstrated for the first time that the dragging parameter of GB edge depends on the shape of the boundary edge components.



Non-stoichiometry, electrowetting and contact interaction of zirconia, titania or hafnia with metal melts

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Introduction/Purpose

Transition metal oxides, in particular titania, zirconia and hafnia, due to high anions mobility can lose oxygen with formation of non-stoichiometry phases and also pass the electric current at high temperature. It influences the properties of materials in particular contact interaction to metals. So the wetting of zirconia, hafnia and titania with inert metal melts (Cu, Ni, Pt, Cu-Ga, Cu-Ge est.) in conditions when high non-stoichiometry of oxides was provided and when current passed through the interfaces was studied.

Methods

Sessile drop wetting study in vacuum, microstructure and X-ray investigation were used. In wetting experiments with high non-stoichiometry oxide samples contacted at the same time with active metal melts (Ti, CuTi, Ni-Ti) to provide the oxygen deficit in substrates and with inert metal melts (Cu, Ni, Pt, Cu-Ga, Cu-Ge est.) In experiments with current metal drops situated between ceramic or ceramic and metal plates connected to current leads.

Results

When inert and active metals contact to ceramic simultaneously inert melts wet the zirconia and the hafnia but not the titania. This effect was explained by dissolution of surplus zirconium and hafnium in melts contributes to the wetting. Titania at contact to active metal reduced to bast oxideand permanent oxygen removal from the samples volume was not provided. Dissolution of zirconium was confirmed for the nickel / zirconia / Ni-Ti samples using the microstructure study and the thermodynamic calculation.

When negative electrode is connected to ceramic wetting significantly improves both for zirconia and titania and hafnia. It was also explained by oxygen depleting of under the current and subsequent dissolution of surplus titanium, zirconium or hafnium in the melt. Results obtained were used to braze zirconia ceramic.

Conclusions

So the non-stoichiometry caused by high anions mobility influences the titania, zirconia and hafnia to metal interaction.

Study on the slag phases and physical properties evolution during foaming practice applied to prolong BOF lining life

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Introduction/Purpose

The maintenance or replacement of the MgO-C refractory lining used in BOF converters represents a high cost in steel production. For this reason, the industry develops different alternative protective practices in order to prolong the campaign of such equipment.

The slag aptitude to achieve a suitable foam that form a protective layer on the MgO-C brick surface is determined by the phases present in the slag and their physical properties evolution at the operating conditions. Also it is relevant to consider the characteristics (thermal and chemical behaviour and structural aspects) of carbonaceous material added.

Methods

In this paper, six slag samples previous and post foaming practice were characterized. The melting behaviour, the viscosity and the surface tension, were determined by experimental tests. The crystalline phases were identified by XRD and correlated with a structural study of the samples carried out by optical and scanning electron microscopy. The evolutions of the present phases in the slag during the foaming practice were predicted by thermodynamic simulation applying FactSage. The thermal behaviour and structural characterization of the carbonaceous materials also provided complementary information to optimize the foaming practice.

Results

All the information obtained allows to determine the foaming index and to identify the operation variables to control the foaming practice. On this base it is possible to the BOF operators to estimate the foaming index on line and to avoid slopping problems.

Conclusions

The foaming practice results in a considerable increase of the MgO-C lining life.

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Surface and bulk properties of liquid Si-M eutectic alloys (M = Co, Ti, Zr)

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Introduction/Purpose

Computational models are enabling the design and manufacture of costless and high quality advanced complex metal-based materials. Since longer, SiC-based composites gain interest for the use in aerospace, automotive, defense, and various engineering applications. In particular, the production of tailored SiC-based composites via reactive infiltration of Si-based alloys into C-based preforms, mainly by assisting computational simulations, is currently one of the main goals of materials design. However, simulation could successfully proceeds if accurate, self-consistent, and reliable thermophysical properties data of liquid infiltrants are introduced as input. For the liquid Si-based alloys, such data are quite scarce and even contradictory due to the high reactivity of the liquid phase with surrounding materials and/or containers at high temperatures [1]

Methods

In recent years, quasi-containerless methods such as the pendant drop technique, have paved the way for limited contact measurement methods allowing precise determination of key surface and bulk properties for this class of alloys, such as surface tension and density [2, 3]. Systematic investigations of thesurface tension and density properties of Si-M eutectic alloys (M = Co, Ti, Zr) have been carried out by the pendant drop method in the temperature range of (T_m+20) ÷1500°C.

Results

The results obtained have been discussed in terms of alloying element (M), operative conditions and considering phenomena (i.e. segregation, mass tranfer, evaporation, etc.) evolving at the liquid/vapour and liquid/solid interfaces under dynamic scenarios. For these reasons, the results have been analyzed by means of different thermodynamic models, e.g. Ideal solution, Quasi-Chemical Approximation (QCA) for regular solution applied to the basic Si-M systems [3].

Conclusions

The alloying element (M = Co, Ti, Zr) weakly influences the surface tension data of Si-rich Si-M eutectic alloys as predicted by theoretical models applied: alloy surface is mainly dominated by Si-segregation.

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Surface properties of liquid Cu-Zr alloys

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Introduction/Purpose

The Cu-Zr is glass forming system and a subsystem of braze materials. Industrial processes, such as for example, casting, joining, crystal growth and liquid phase sintering involve the presence of the liquid phase and thus, the knowledge of the surface properties related to processed materials and modelling of microstructural evolution during solidification are of great importance. In the present work the surface tension and surface segregation of liquid Cu-Zr alloys [1] have been analysed and the new surface tension experimental data were determined.

Methods

To measure the density and surface tension of liquid Cu-Zr alloys, the contact heating sessile drop method was applied [2]. For each alloy, the measurements were performed under Ar-H2 atmosphere for the temperatures ranging between the melting point (Tm) and (Tm + 200 °C). After each experiment, the samples were analyzed by SEM-EDX.

Results

The Compound Formation Model (CFM) and Quasi Chemical Approximation for regular solutions (QCA) were used to calculate the surface tension isotherms. The experimental surface tension data of liquid Cu-Zr alloys obtained in the present work were compared to available literature data as well as to the model predicted values. In particular, the new experimental data on the Cu50Zr50 alloy was compared to the corresponding data recently obtained by an electromagnetic levitator (EML) under microgravity aboard the International Space Station (ISS) [3].

Conclusions

The new surface tension experimental data of liquid Cu-Zr and datasets available in literature differ up to 5%. From the theoretical point of view, the choice of the surface tension reference data used as input to calculate the surface tension isotherms is one of critical points for evaluation of experimental data reliability.

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The effect of the third component on the fraction of wetted grain boundaries in the alloy Zr-2.5 wt.% Nb

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Introduction/Purpose

Zirconium alloys are widely used in nuclear reactors, due to their high corrosion resistance. Zirconium is an extremely successful material due to its ease of preparation, good ductility, resistance to radiation damage, low thermal neutron capture and excellent corrosion resistance. The aim of the work was to investigate the effect of temperature treatment and the third component on the morphology of the alloy Zr - 2.5 wt.% Nb.

Methods

To study the microstructure by the method of induction melting in vacuum, three-component alloys Zr - 2.5 wt.% Nb – X (where X is 1 wt.% Fe or Cr) were prepared. Washers 5 mm thick were cut from the obtained rods. Then, the polycrystalline samples were sealed in quartz ampoules (P = 4×10^4 Pa) and annealed in the two phase region (aZr) + (bZr, bNb) of the bulk phase diagram Zr – Nb. After quenching the water, the microstructure of the polycrystalline samples was examined using optical and scanning electron microscopes.

Results

In figure shows the temperature dependences of the fraction of wetted GBs in Zr-2.5 wt.% Nb, Zr-2.5 wt.% Nb-1 wt.% Fe, and Zr - 2.5 wt.% Nb - 1 wt.% Cr.

Conclusions

All temperature dependences have a parabolic shape. Iron increases the proportion of wetted grain boundaries compared to the original two-component alloy Zr - 2.5 wt.% Nb. By adding a third component (chromium), it is possible to maintain a high proportion of wetted grain boundaries in a wide temperature range (more than 100°C).



The role of torque terms in capillary equilibrium along triple junctions in polycrystalline copper

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Introduction/Purpose

One of the most popular methods for grain boundary (GB) energy determination involves the use of the Herring equation, which describes the capillary equilibrium along junction of three GBs. This equation includes the so-called torque terms, which are related to the variation of GB energy with GB plane orientation. It is often accepted that torque terms are negligible for all GBs except for coherent twins, which makes it possible to use the Herring equation in a simplified form [1]. However, this assumption has not yet been unequivocally confirmed experimentally.

Methods

We have measured dihedral angles in GB grooves formed after 6 h at 1000 °C under flowing H_2 for 18 GBs which forms 6 triple junctions in polycrystalline copper foil. GB energies were calculated under the assumption of isotropic surface energy of solid copper. Capillary equilibrium along triple junctions was analyzed in detail using the complete Herring equation and values of torque terms were estimated. Misorientation and GB plane orientation for studied GBs was determined on the basis of SEM and EBSD data. GB energies were calculated using the 5DOF function proposed in [2] and compared with experimentally obtained values.

Results

The average value of torque terms was found to be over 15% of the GB energy, despite the fact that most of considered GBs are of general type. Large torque term values could be explained by the presence of metastable configurations of GBs due to unrelaxed microscopic degrees of freedom.

Conclusions

Thus, the torque terms must be taken into account even for general-type grain boundaries in FCC metals at 0,95Tm.

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Wettability gradient enhanced loop heat pipe for portable electronics

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Introduction/Purpose

With the rapid development of techniques in the microelectronic technology and high-density packaging of electronic components, portable devices such as smartphones, tablets, and notebook computers, are being developed with high performance, light weight and miniaturization. High-flux heat dissipation in a limited space is encountered in many electronics applications. To solve the heat problems, cooling solutions such as high conductivity materials, phase change materials, and small heat pipe technologies, have focused on distributing heat as evenly as possible. The heat-spreading performance of high conductivity materials, such as graphite sheets is limited by their thermal conductivity. Thin-layered phase change materials cannot sufficiently respond to the large degree of heat generation. The use of heat pipe technology, which exhibits heat-transport performance superior to that of high conductivity materials, can offer effective solutions for thermal diffusion within portable devices.

Methods

In this work, we demonstrate a new cooling solution for the high-flux heat dissipation of portable electronics. We fabricated a prototype model of the loop heat pipe by a chemical-etching and surface treatment process for thin copper plates. The gradient in wettability (from superhydrophobic to hydrophilic) along the condenser line was fabricated by the formation of self-assembled structure gradient via a rapid electrodeposition process. A ceramic heater was utilized as the heat source. Several thermocouples were attached to the loop heat pipe to measure the temperatures at different locations. The surface temperature profile was captured with a Flir i60 infrared camera.

Results

Experimental results showed that the surface wettability remarkably influenced the fluid motion and thermal performance of loop heat pipe. The circulation of the working fluid in the loop heat pipe was greatly enhanced by the wettability gradient along the condenser line.

Conclusions

The experimental results demonstrated that the present loop heat pipe is a powerful cooling solution to portable electronics.

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Figure 1. Schematic of the loop heat pipe.

Wetting of different grain boundary types in an industrial Mg cast alloy

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Introduction/Purpose

The alloy EZ33A is an alloy based on the Mg-Zn system, which is used in the aerospace industry. In the cast state, this alloy demonstrates low microporosity, good weldability, and creep resistance up to 250 ° C. But with good performance of some properties, it has a low ductility at room temperature. The reason for low plasticity is the formation of intermetallic compounds at the grain boundaries. In order to improve the structure of this alloy and its mechanical properties, the goal was set: to experimentally investigate the grain boundary wetting phase transition of α -Mg/ α -Mg grain boundaries by the second phase.

Methods

After experimental annealing and metallographic preparation, we used methods such as scanning electron microscopy, transmission electron microscopy, electron backscattered diffraction, and Vickers hardness measurements.

Results

Later analyzed the data, we proved the existence of a phase transition by wetting the α-Mg grain boundaries with the second liquid phase. Following series of annealing, the temperature of the eutectic transformation of the magnesium alloy EZ33A and the temperature of the onset of the wetting phase transition were determined.

Conclusions

In order to increase the ductility of the alloy at room temperature, an optimal heat treatment sequence was identified.

Selected references

The work was performed with the financial support of the Russian Foundation for Basic Research (Project # 18-33-00473).

Wetting of individual Sn/Sn grain boundaries by the Zn-rich melt

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Introduction/Purpose

The wetting phase transition is an interesting surface effect investigated by the modern material science. It is important not only as a fundamental grain boundary effect that has a strong influence on the total energy of metallic systems, but also for industrial applications, such as welding, soldering or structure formation at elevated temperatures. It is well known that the wetting is in most cases a surface phase transition of 1st order. The temperature dependence of the wetting contact angle has usually a discontinuity at the wetting temperature. However, the wetting can be a 2nd order phase transition. It has been shown in the literature that the temperature derivative of the wetting contact angle of liquid (Al) on Zn/Zn grain boundaries changes continously. The authors estimated that the wetting of Sn/Sn grain boundaries by (Zn) could exhibit a 2nd order behavior too.

Methods

Bicrystals with individual Sn/Sn coincidence grain boundaries were produced. The surface of the samples was dipped into eutectic Sn–Zn melt. All the samples were encapsulated in ampoules with residual pressure of 4*10⁻⁴ Pa. The ampoules were annealed at different temperatures to achieve different wetting states with different contact angle values. The samples were then investigated on a scanning electron microscope.

Results

All grain boundaries were wetted at about 215° C well below the melting temperature of Sn (T_m =231°C). As it was expected, the contact angle decreases with increasing temperature and its temperature derivative changes continuously. This proves that the wetting phase transition of Sn/Sn grain boundaries by (Zn) is a 2nd order phase transition.

Conclusions

As expected, the 2nd order wetting phase transition has been found on individual coincidence site lattice Sn/Sn grain boundaries wetted by Sn-Zn eutectic.

Wetting of different grain boundary types in an industrial Mg cast alloy

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Introduction/Purpose

The EZ33A alloy is a magnesium cast alloy used in the industry. Low microporosity, good weldability and creep resistance up to 250 °C are the most important properties of this alloy. Nevertheless, the ductility of this alloy at ambient temperature is very poor and limits the range of machining method applicable. According to the literature the poor ductility is caused by the hard and brittle intermetallic phase that covers the grain boundaries. The investigation of wetting transition on different grain boundaries will explain how to increase the ductility by controlling the number of boundaries wetted by the intermetallic phase.

Methods

The samples of EZ33A were annealed at different temperatures between solidus and liquidus to obtain different wetting states of the system and quenched. After metallographic preparation, the samples were investigated in the scanning electron microscope (SEM) with the electron backscattering diffraction method (EBSD). The EBSD data was analyzed.

Results

Under annealing, the Mg/Mg grain boundaries in the polycrystalline samples become wetted by the liquid phase (the Mg₁₂RE intermetallic phase in the quenched state, where RE stays for rare-earth metals). The figure shows an SEM micrograph of an as-cast EZ33A structure. The bright gray phase - Mg₁₂RE intermetallic. The dark gray grains - α-Mg phase. 75% of grain boundaries are wetted. As a result, the authors evaluated the whole angular spectrum of grain boundaries found in this alloy in a stable state concerning the wetting temperatures of these grain boundaries and their crystallographic structure. The biggest fraction of the spectrum with the low grain boundaries with low energy have high wetting temperatures and occupy a narrow fraction of the spectrum.

Conclusions

To increase the ductility one has to decrease the number of wetted boundaries and/or increase the number of special boundaries.

Selected references

The work was performed with the financial support of the Russian Science Foundation (Project # 18-72-00243).



Effect of thermal treatment on morphology of phase (bTi) in Ti6Al4V Alena Gornakova^{*} Sergei Prokofjev Institute of Solid State Physics of the Russian Academy of Sciences, Chernogolovka, Russian Federation *alenahas@issp.ac.ru

Introduction/Purpose

The alloy Ti6Al4V is widely used in aerospace engineering, machine building and shipbuilding, and has a wide biomedical use. This is due to the possibility of forming a wide range of its mechanical characteristics (from high heat resistance to superplasticity) with the help of various thermal and thermo-mechanical treatments. This is due to a change in the quantitative ratio, morphology and dispersion of (α Ti) and (β Ti) phases in the bulk and at the grain boundaries. The purpose of this work is to study the effect of annealing parameters in the (a+b) region on the morphology and dispersion (β Ti) of the phase at the grain boundaries in (α Ti) in the Ti₆Al₄V alloy.

Methods

Studies were conducted on industrial alloy Ti_6AI_4V (bar with a diameter of 25 mm). Subsequent tests showed structural and chemical homogeneity of the rod. On an electric spark machine, the bar was cut into washers 5 mm thick, which were then cut into four equal parts. Then they were sealed in quartz ampoules and annealed in vacuum at a residual pressure of 4×10^{-4} Pa. Annealing was performed at temperatures of 660-900°C (average duration of annealing 720 hours), i.e. in the ($\alpha + \beta$) region of the Ti–V–AI phase diagram.

Results

The figure shows the SEM micrograph of the studied alloy annealed at $T=800^{\circ}$ C for 840 hours (GB_w - wetted grain boundary (GBs), GB_{ww} – not wetted).

Conclusions

Conclusion: It is shown that the fraction of grain boundaries (aTi) fully covered (bTi) with the phase increases with temperature. Below a temperature of approximately 650°C, all grain boundaries in (α Ti) are free from a continuous layer (bTi). Since the ratio of the grain boundaries in (α Ti) and interphase boundaries (α Ti)/(bTi) significantly changes with an increase in the annealing temperature, we can expect that these changes will affect the strength and ductility of the annealed Ti₆Al₄V alloy.

