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Перспективные материалы с иерархической структурой для новых технологий и надежных конструкций
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components – модель TEC). Рассматривая исследуемый материал в области фазового перехода как смесь фаз низкого и высокого давления, модель TEC позволяет достоверно описывать, в том числе, и область полиморфного фазового перехода [3]. Результаты моделирования позволяют описывать термодинамические параметры смеси в том числе с компонентами, испытывающими фазовый переход при высоких динамических нагрузках. Для расчета ударно-волнового воздействия на такие смеси используются параметры уравнения состояния только их компонентов. Предполагается, что начало фазового перехода компонентов при ударно-волновом нагружении происходит при тех же параметрах, что и в чистых веществе.

Наличие экспериментальных данных позволило оценить достоверность расчетов с учетом предположений, использовавшихся в модели. Результаты моделирования хорошо соответствуют известным данным различных авторов, полученным на основании экспериментов для кварца, нитридов, висмута, графита, а также для смесей кварца с различными материалами [3]. Показано, что модель TEC позволяет моделировать термодинамические параметры смесей при ударно-волновом нагружении, при этом в состав исследуемой смеси могут входить несколько компонентов, испытывающих фазовый переход. Расчетные термодинамические параметры соответствуют данным, определенным на основании экспериментов для смеси AlN с оксидом магния MgO, а также для смеси Si_3N_4 с бромидом калия KBr.

Полученные результаты показывают перспективность использования материалов с фазовым переходом в виду того, что они дают возможность изменять значения температуры в более широком диапазоне значений, расширяя область достижимых термодинамических параметров

Литература:

1. Кинеловский С.А., Маевский К.К. Модель поведения алюминия и смесей на его основе при высоком динамическом воздействии //ТВТ. 2014. Т. 52. № 6. С. 843-851.
2. Кинеловский С.А., Маевский К.К. Оценка термодинамических параметров ударно-волнового воздействия на высокопористые гетерогенные материалы // ЖТФ. 2016. Т. 86. № 8. С. 125-130.
3. K. K. Maevskii, S.A. Kinelovskii Thermodynamic parameters for mixtures of quartz under shock wave loading in views of the equilibrium model // AIP Conference Proceedings. 2015. V. 1683. P. 020132 (1 - 4).

PLASTIC DEFORMATION NUCLEATION IN ELASTICALLY LOADED CuNi ALLOY DURING NANOINDENTATION

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Nowadays the production of different micro- and nanoelectromechanical systems is being actively developed. Many components of such systems while in operation are in mechanical contact with each other. Understanding the mechanisms of their interaction on the atomic scale is important for improvement of mechanical properties of available systems and for development of new ones. Along with experimental research, computer simulation of the behavior of materials during nanoindentation has been actively developed in the last decades. In the context of the foregoing, the objective of the present work is the study of the features of nucleation and development of plastic deformation in previously elastically deformed CuNi crystallites during nanoindentation. The many-body potential in approximation of the embedded atom method was used to describe the interatomic interactions in simulated samples. The calculations were performed using the LAMMPS package. Identification of structural defects was conducted by common neighbor analysis.

Simulation showed that the plastic deformation under uniaxial tension of the crystallites begins to nucleate at the free surface. It was found that the character of the nucleation of the plastic deformation depends on the stoichiometric composition. So, the extrinsic and intrinsic stacking faults are formed at the nucleation of plastic deformation in the crystallites with small concentrations of nickel. The twinning mechanism starts to make sufficient contribution to plasticity at high concentrations of nickel. Threshold values of deformation for pure copper and nickel are significantly different. Since the CuNi alloy is a solid solution, it can be expected that the threshold deformation will change in proportion to the concentration of the elements. Indeed, the threshold deformation is almost linearly dependent on the concentration of the second element.

Based on the obtained threshold values of deformation, four values were chosen for each concentration of nickel, including zero and close to the threshold. The results of simulation showed that the threshold value of indentation, at which plastic deformation begins to nucleate, decreases with increasing elastic pre-stretching of copper samples. This behavior at nanoindentation is also characteristic for CuNi alloys and pure nickel. As in the case of uniaxial tension, stacking faults are formed in the indented crystallites. It should be noted that at small values of the elastic pre-stretching, the defect nucleation occurs in the region where indenter contacts with the crystallite. However, in the case of elastic pre- stretching close to the threshold value, the region of defect nucleation is shifted. The attraction of the contact zone to indenter results in a distortion of a neighboring region and leads to the appearance of excess stresses. As a result, the structural defects begin to nucleate in distorted region. The formed defect structure in this case is more complex than for small elastic pre-stretching.

COMPUTATIONAL STUDY OF THE MECHANICAL BEHAVIOR OF STEEL PRODUCED BY SELECTIVE LASER MELTING

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Selective laser melting (SLM) is the metal additive manufacturing technology that employs a laser beam to heat and melt a bed of powder to produce metal parts of highly complex geometries in a layer-by-layer fashion. Given that SLM is a complex multiphysical process, it is a challenge to understand processing-microstructure-property relationships in a material so produced. In this work, a two-dimensional numerical analysis of the evolution of grain structure observed during SLM and of the mesomechanical behavior of additive manufactured specimens is performed.

Cellular automata finite-difference (CAFD) model is developed to simulate the evolution of grain structure. A heat equation is solved with the use of the classical FD scheme. The CA model for the simulation of microstructural evolution is based on the approach put forward by Rappaz and Gandin. The double ellipsoid heat source model is adopted to describe the heat input during SLM process.

The process of selective laser melting is simulated as follows. First, the polycrystalline steel substrate is generated. Then a powder layer is deposited on the substrate and is locally melted by the laser beam, which moves in a certain predetermined way. On laser irradiation and cooling of the powder layer, another powder layer is deposited on the resulting solid structure and the procedure is repeated until a predetermined number of layers is reached.

Then the resulting microstructure is cut off from the substrate and subjected to uniaxial tension. An elastoplastic constitutive model including isotropic strain hardening is used to describe the mechanical response of additive manufactured specimens on the mesoscopic