

ENHANCEMENT OR SUPPRESSION OF STRUCTURAL PHASE TRANSITION IN $Ti_{1-x}Al_xN$ BY PRESSURE AND STRESS

Svetlana A. Barannikova^{1,2}, Albina M. Zharmukhambetova³, Anton Yu. Nikonov⁴,
Andrey I. Dmitriev⁵, Alena V. Ponomareva⁶ and Igor A. Abrikosov^{7,8}

¹Institute of Strength Physics and Materials Science, Siberian Branch of Russian Academy of Science, Tomsk, Russia, bsa@ispms.tsc.ru, <http://www.ispms.ru/>

²Tomsk State University, Tomsk, Russia, bsa@ispms.tsc.ru, <http://persona.tsu.ru/>

³Tomsk State University, Tomsk, Russia, almura@sibmail.com, <http://persona.tsu.ru/>

⁴Institute of Strength Physics and Materials Science, Siberian Branch of Russian Academy of Science, Tomsk, Russia, nikonov@usgroups.com, <http://www.ispms.ru/>

⁵Institute of Strength Physics and Materials Science, Siberian Branch of Russian Academy of Science, Tomsk, Russia, andr23@yahoo.com, <http://www.ispms.ru/>

⁶National University of Science and Technology MISIS, Moscow, Russia, alenaponomareva@yahoo.com, <http://www.misis.ru/>

⁷Linköping University, IFM, Campus Valla, 581 83, Linköping, Sweden, igor.abrikosov@ifm.liu.se, <http://www.ifm.liu.se/theomod/theophys/>

⁸National University of Science and Technology MISIS, Moscow, Russia, iabrikosov@misis.ru, <http://www.misis.ru/>

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Multiscale approach allows one to capitalize on the success of the modern first-principles simulations, and to use quantum mechanics calculations to determine essential materials parameters for the use in higher-level models. We demonstrate that by means of computer experiment it is possible to create data-bases of relevant materials parameters which are difficult, expensive or impossible to obtain in physical experiments. Example of this approach is given for Ti and Zr- based alloys. They are attractive for technological applications. Hexagonal closed packed (hcp)Zr-based alloys represent a material system widely used in nuclear energy applications, e.g. as fuel cladding materials. hcp Ti alloys do not have high strength, but they show strong hardening during cold deformation. Their disadvantage is reduced technological plasticity. With the aim to assist knowledge based design of new Ti and Zr-based alloys, we carry out *ab initio* simulations of effect of chemical composition and pressure on mixing enthalpies and elastic properties of binary and multicomponent Ti-Al-V-Mo and Zr-Nb systems and determine conditions for their thermodynamic and mechanical stability. Using the calculated parameters, we establish a significant correlation between the product of the macroscopic parameters of localized plastic flow auto-waves in deforming alloys, their length and propagation rate and the product of the microscopic (lattice) parameters of these materials, the spacing between close-packed planes of the lattice and the rate of transverse elastic waves. We therefore demonstrate that *ab initio* simulations can be used for the prediction of parameters of localized plastic flow auto-waves in deforming alloys.