Ab initio theory of alloys: new possibilities for materials design.

I. A. Abrikosov

[1]*Department of Physics and Measurements Technology, Linköping University, Linköping, Sweden*

We will review recent developments in the field of *ab initio* electronic structure theory and its application for studies of complex alloy systems. Basic ideas behind state-of-the-art techniques for first-principles theoretical simulations of the phase stabilities and properties of intermetallic compounds and alloys based on the density functional theory will be outlined. We will concentrate on methods that allow for an efficient treatment of disorder effects [1,2], and illustrate their predictive power with examples.

Three major factors that determine the structure of a material are the valence electron concentration, the difference in electronegativity and the difference in size between its constituents. The ability of the first-principles theory to describe the phase transitions in complex materials upon the change of the electron concentration, and to understand their origin, will be illustrated by the study of anomalous stability of ferritic low Cr steels against the radiation damage [3]. Moreover, we will show that the electronic structure variation with alloy concentration plays the decisive role in the mixing and decomposition thermodynamic of hard coating nanocomposite thin films based on transition metal nitrides [4]. The ability of the *ab initio* materials design will be illustrated by the theoretical optimization of ionic conductivity in doped ceria [5].

[1] I. A. Abrikosov, A. M. N. Niklasson, S. I. Simak, B. Johansson, A. V. Ruban, and H. L. Skriver, Phys. Rev. Lett. **76**, 4203 (1996).
[2] L. Vitos, I. A. Abrikosov, and B. Johansson, Phys. Rev. Lett. **87**, 156401 (2001).
[3] P. Olsson, I. A. Abrikosov, and J. Wallenius, Phys. Rev. B **73**, 104416 (2006).
[4] B. Alling, A. V. Ruban, A. Karimi, O. E. Peil, L. Hultman, and I. A. Abrikosov, Phys. Rev. B (to be published).
[5] D. A. Andersson, S. I. Simak, N. V. Skorodumova, I. A. Abrikosov, and B. Johansson, "Optimization of ionic conductivity in doped ceria", PNAS **103**, 3518 (2006).