Ab-initio Simulation of Complex Materials Processes: Grain Boundary Cohesion, Diffusion, Phase Diagrams, Solubility Products in Steels and Gate Stack Modeling

Walter Wolf
Materials Design, Le Mans, France, and Angel Fire, (NM) USA

Computer simulation of materials processes and computational property prediction have become a widely accepted resource in the industrial R&D process, complementing and aiding experimental techniques. Applications range from large-scale computational materials prescreening for identification of most promising candidates to property calculation focused on and enabling interpretation of particular measurements. Frequently, the most promising and cost-effective research strategy is a combined experimental and theoretical approach. An effective research process requires access to materials databases, model building capabilities, automated simulation and analysis tools, as well as a flexible infrastructure to distribute computational tasks on distributed compute resources, all of which have been integrated in the MedeA software environment.

The capabilities of modern ab-initio based simulation techniques in industrial research in several different fields of application are reviewed. In stress corrosion cracking and materials fatigue, the segregation of impurities to grain boundaries in nickel and zirconium and their effect on grain boundary cohesion is investigated from first principles[1]. Temperature effects and thermal expansion are included by ab-initio calculation of lattice dynamics enabling within the framework of transition state theory the accurate prediction of temperature dependent diffusion coefficients in bulk materials[2] and grain boundaries[3]. Taking into account configurational entropy by a simple independent two-site model, in addition to vibrational terms, enables quantitative prediction of the P-T-X phase diagram of the yttrium-hydrogen system. Aiming at improved mechanical properties of high-chromium ferritic steels by precipitation hardening, temperature dependent solubility products are predicted from first principles to identify suitable steel compositions for casting. As an application in electronic industries, the advanced miniaturization in microelectronic device technology and progress in quantum physical methods nowadays allow ab initio modeling of effective work functions in gate stacks approaching realistic device dimensions[3,4].

References:

1. M. Christensen, T. M. Angeliu, J. D. Ballard, J. Vollmer, R. Najafabadi, E. Wimmer, J. Nucl. Mater. **404**, 121 (2010)
2. E. Wimmer, W. Wolf, J. Sticht, P. Saxe, C. B. Geller, R. Najafabadi, and G. A. Young, Phys. Rev. B **77**, 134305 (2008)
3. E. Wimmer, R. Najafabadi, G. A. Young Jr., J. D. Ballard, T. M. Angeliu, J. Vollmer, J. J. Chambers, H. Niimi, J. B. Shaw, C. Freeman, M. Christensen, W. Wolf, and P. Saxe, J. Phys.: Condens. Matter **22**, 384215 (2010)
4. C. L. Hinkle, R. V. Galatage, R. A. Chapman, E. M. Vogel, H. N. Alshareef, C. Freeman, E. Wimmer, H. Niimi, A. Li-Fatou, J. B. Shaw, J. J. Chambers, Appl. Phys. Lett. **96**, 103502 (2010)