Condensed Matter Seminar
Institute of Physics of Materials AS CR

on **November 20, 2012** (Tuesday) at **10:00 am**
in the lecture room (4th floor)
of the Institute of Physics of Materials AS CR, Žižkova 22, Brno

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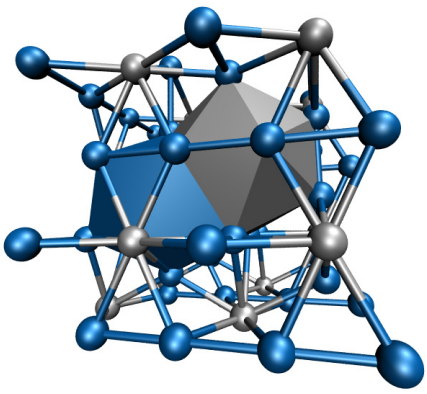
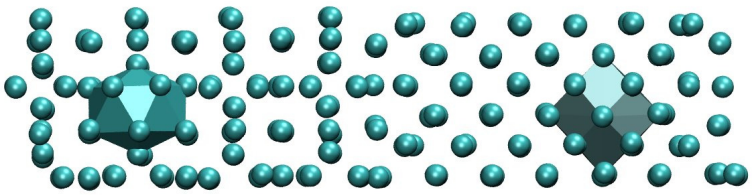
From density-functional theory to analytic bond-order potentials: Application to topologically close-packed phases

Topologically close-packed (TCP) phases play in important role in many modern alloys and steels. While particular TCP phases are desirable in precipitate-hardened steels, the precipitation of TCP phases in single crystal Ni-based superalloys has a detrimental effect on the mechanical properties. In order to gain a microscopic understanding of the factors that control TCP phase stability, we coarse-grain the electronic structure from density functional theory (DFT) to tight-binding to bond-order potentials (BOPs). The analytic BOP depends explicitly on the valence of the transition metal (TM) elements and accounts for charge transfer and magnetic contributions to the binding energy. The analytic BOPs may then by employed in large-scale atomistic simulations. The prediction of the BOPs is compared to extensive high-throughput DFT calculations for the TCP phases A15, C14, C15, C36, mu, sigma, and chi, which confirm the well known trend of structural stability of TCP phases with average d-band filling. The structural trend across the non-magnetic 4d and 5d TM is then analyzed with the analytic BOPs. This enables us to relate the structural stability of TCP phases to the local topology of the atomic structure and bandfilling. We then apply the analytic BOPs in large-scale atomistic simulations in order to investigate the atomic structure and energetics of interfaces between the cubic phases BCC and FCC and the TCP phases sigma and A15. We show that recently parametrised BOPs for refractory elements are suitable for the description of TCP phases at elevated temperatures and report on the first dynamic simulations of interfaces between cubic phases and TCP phases.





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