MM 5: Materials Design I

Time: Monday 10:15–11:45   Location: IFW D

MM 5.1   Mon 10:15   IFW D

Using ab initio calculations in designing bcc Mg-Li alloys for ultra light-weight applications — William Art Counts, •Martin Friák, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

Ab initio calculations are becoming increasingly useful to engineers interested in designing new alloys because these calculations are able to accurately predict basic material properties only knowing the atomic composition of the material. In order to explore the suitability of this approach in identifying potential candidates for ultra-light-weight applications we studied bcc Mg-Li alloys. In a first step, the fundamental physical properties (like formation energy and elastic constants) of an extensive set of bcc Mg-Li compounds are calculated using density-functional theory (DFT) and compared with available experimental data. These DFT-determined properties are in turn used to calculate engineering parameters like (i) specific Young's modulus (Y/ρ) or (ii) bulk over shear modulus ratio (B/G) differentiating between brittle and ductile behavior. In a second step, these engineering parameters are used to identify alloys that have optimal mechanical properties needed for a light-weight structural material. It was found that the stiffest bcc magnesium-lithium alloys contain about 70 at.% Mg while the most ductile alloys have 0-20 at.% Mg. An Ashby map containing Y/ρ vs. B/G shows that it is not possible to increase both Y/ρ and B/G by changing only the composition of a binary alloy (W. A. Counts, M. Friák, D. Raabe, J. Neugebauer, Acta Mater 57 (2009) 69).

MM 5.2   Mon 10:30   IFW D

Effect of interstitial carbon on the magnetic structure of fcc iron: Towards an ab-initio understanding of austenitic steels — •Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH,Max-Planck-Straße 1,40237 Düsseldorf,Germany

It is known that the mechanical properties of austenitic steels strongly depend on their carbon content. However, the impact of carbon on the stability of the complex magnetic structure of the austenitic iron host is still controversially debated in the literature. Therefore, we present a systematic ab initio investigation of the interaction of interstitial C with the magnetic structure of austenitic iron. Our results are obtained within the DFT-GGA approach, making use of the PAW method and the collinear approximation for the magnetic moments. We find a principle preference of the C atoms for a FM environment. However, this yields only for very high carbon concentrations (>10 at.%) to a preference of the FM structure for the entire austenitic crystal. For lower concentrations (< 3 at.%), the anti-ferromagnetic double layer (AFMD) structure, representing the magnetic ground-state of pure fcc-Fe, remains the most stable phase. The transition from AFMD to FM ordering takes place at 8 at %, is surprisingly sharp, and a collective phenomenon of all C atoms in the Fe host matrix.

MM 5.3   Mon 10:45   IFW D

DFT calculations on the Fe/ZrO2 system — •Kutzner Jürgen and Kortus Jens — TU Bergakademie Freiberg, Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg, Germany

The interface Fe/ZrO_2 has been investigated in view of its interface structure and mechanic properties by means of density functional theory calculations.
The pure phases of iron and zirconium dioxide have been studied first as point of reference. The results include phase transitions and bulk-moduli which compare well with experimental data. Further, we have examined possible structural models of simple epitactic phases of Fe and ZrO_2. These models will be discussed in terms of their relative stability. At a next step iron is replaced by more realistic approximations of steel. The influence of different chemical composition on interface structure and materials properties is investigated.
We would like to thank the DFG for financial support within SFB 799: TRIP-Matrix-Composite.

MM 5.4   Mon 11:00   IFW D

The free energy of iron: Integrated ab initio derivation of vibrational, electronic, and magnetic contributions — •Fritz Körmann, Alexey Dick, Blazej Grabowski, Tilmann Hickel, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, D-40237, Düsseldorf, Germany

In this talk we present our recently developed [1] integrated ab initio approach including vibrational, electronic, and magnetic contributions to derive the thermodynamic properties of ferromagnetic bcc iron. The quasiharmonic approximation and finite-temperature density functional theory are employed to account for vibrational and electronic excitations. In particular the magnetic contribution to the free energy, which is of crucial importance for the structural phase stability in iron, will be discussed. This contribution has been derived by generalizing an existing many-body theory for the S=1/2 ferromagnet to arbitrary spin quantum numbers and to non-collinear magnetic configurations where the latter is of particular importance for the fcc phase. This approach has lead to an excellent agreement with available experimental data for bcc iron.
[1] F. Körmann, A. Dick, B Grabowski, B. Hallstedt, T. Hickel, and J. Neugebauer, Phys. Rev. B 78, 033102 (2008).

MM 5.5   Mon 11:15   IFW D

Ab initio up to the melting point: Anharmonicity and vacancies in aluminum — •Blazej Grabowski, Lars Ismer, Tilmann Hickel, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Düsseldorf, Deutschland

At elevated temperatures, the heat capacity of metals strongly deviates from the harmonic prediction. This was pointed out long ago[1] and various explanations have been considered. Recently, ab initio calculations showed that a dominant part can be explained by quasiharmonic and electronic excitations.[2] However, the *detailed* balance of further contributions, such as explicit anharmonicity and vacancies, is not clarified yet even for simple elementary metals. Aluminum is a prototypical example. Even though intensively studied, the ambiguous experimental situation has made a classification of the mechanisms impossible.

To resolve the situation, we have calculated the full volume and temperature dependent *ab initio* free energy surface employing density-functional theory. In particular, we have included anharmonic and vacancy contributions using numerically highly efficient methods to coarse grain the configuration space. To obtain accurate vacancy energies, we have included the full spectrum of excitations: quasiharmonic, electronic, and explicitly anharmonic. The results are in contradiction to common belief, nevertheless the essential physics can be captured by a simple model.
1. M. Born and E. Brody, Zeitschrift für Physik 6, 132 (1921).
2. B. Grabowski, T. Hickel, and J. Neugebauer, Phys. Rev. B 76, 24309 (2007).

MM 5.6   Mon 11:30   IFW D

Theoretical multi-physics approaches to solid-solution strengthening of Al — •Duancheng Ma, Martin Friák, Dierk Raabe, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Strasse 1, 402 37, Düsseldorf, Germany

The strengthening of soft metallic materials has a long tradition and is an important metallurgical topic since the time when ancient smiths forged the first swords. Intense materials research revealed a combination of three mechanisms as decisive for solid-solution strengthening phenomena: (i) the size mismatch of components (Mott and Nabarro's parelastic concept [1]), (ii) the elastic modulus mismatch of atoms (Fleischer's dielastic contribution [2]), and (iii) the concentration of solutes (statistical concept of Friedel [3] and Labusch [4]). Combining density functional theory calculations and linear-elasticity theory, the key parameters that are essential for the classical strengthening theories are determined in order to test them and identify their possible validity limits. The strengthening of fcc aluminium is chosen as an example and a series of binary systems Al-X (with X = Ca, Sr, Ir, Li, Mg, Cu) was considered. Comparing our results with those obtained by applying classical theories we find clear deviations. These deviations originate from non-classical lattice distortions due to the size mismatch of solute atoms in their first coordination shells.
1. N. F. Mott and F. R. N. Nabarro, Proc. Phys. Soc. **52**, 86 (1940).
2. R. L. Fleischer, Acta. Metall. **9**, 996 (1961).
3. J. Friedel, Dislocations (1964).

4. R. Labusch, Phys. Stat. Sol. **41**, 659 (1970).