R. Lizárraga et al., J Material Sci Eng 2018, Volume 7
DOI: 10.4172/2169-0022-C8-113

Stacking fault energies for fcc co-based binary alloys: a first principles study

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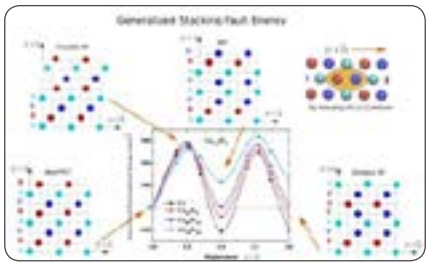
The stacking fault energy is closely related to structural phase transformations and can help to understand plastic deformation mechanisms in materials. Here we perform first principles calculations of the stacking fault energy in the face centered cubic (fcc) Cobalt-based binary alloys $Co_{1-x}M_x$, where M = Cr, Fe, Ni, Mo, Ru, Rh, Pd and W. We investigate the concentration range between 0 and 30 at. % of the alloying element. The results are discussed in connection to the phase transition between the low-temperature hexagonal close packed (hcp) and the fcc structures observed in Co and its alloys. By analyzing the stacking fault energies, we show that alloying Co with Cr, Ru, and Rh promotes the hcp phase formation while Fe, Ni and Pd favor the fcc phase instead. The effect of Mo and W on the phase transition differs from the other elements, that is, for concentrations below 10 % the intrinsic stacking fault energy is lower than that for pure fcc Co and the energy barrier is higher, whereas above 10\% the situation reverses. We carry out also thermodynamic calculations using the Calphad method. The trends of the ab initio stacking fault energy are found to agree well with those of the molar Gibbs energy differences and the phase transition temperature in the binary phase diagrams and give a solid support for the phase stability of these alloys.



Recent Publications

1. L. Tian, R. Lizárraga et al. (2017) A First Principles Study of the Stacking Fault Energies for fcc Co-based Binary Alloys. Acta Materialia 136:215-223.
2. R. Lizárraga et al. (2017) First Principles Theory of the hcp-fcc Phase Transition in Cobalt. Scientifc Reports 7:3778
3. R. Lizárraga (2016) Structural and magnetic properties of the Gd-based bulk metallic glasses GdFe2, GdCo2, and GdNi2 from first principles. Phys. Rev. B 94:174201.
4. M. Araujo et al. (2014) Disorder-induced room temperature Ferromagnetism in Glassy Chromite. Scientific Reports 4:4686.
5. A. Lindmaa, R. Lizárraga et al. (2013) Exchange interactions in paramagnetic amorphous and disordered crystalline CrN-based systems. Phys. Rev. B 88:054414

Biography

R. Lizárraga is a researcher at the department of Materials Science and Engineering at the Royal Institute of Tecknology in Seden. She has large expertise in ab initio calculations. She has great knowledge on magnetism of transition metals and rare earth systems. She has also studied materials with lack of periodic order, such as glassy systems. She has used an ab-initio method, the stochastic quenching method to study the amorphous structure of glassy materials. Recently she has studied the problem of Co substitution in cemented carbides. By studying stacking fault energies she has been able to identified possible alternative substitutions for Co, which is an important industry problem..

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