Elastic constants of random fcc Ti-Al alloy from SQS and CPA calculations

•***Li-Yun Tian*** [1] ***Qing-Miao Hu*** [2] ***Levente Vitos*** [1,3,4]

[1] *Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology (KTH), Stockholm, Sweden*
[2] *Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China*
[3] *Department of Physics and Astronomy, Division of Materials Theory, Uppsala University, Box 516, SE-75121, Uppsala, Sweden*
[4] *Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, P.O. Box 49, H-1525 Budapest, Hungary*

Special quasi-random structure (SQS) and coherent potential approximation (CPA) are techniques widely employed in the first-principles calculations of random alloys. Here we scrutinize these approaches by focusing on the local lattice distortion (LLD) and the crystal symmetry effects. We compared the lattice parameters, mixing energy, and elastic constants obtained from SQS and CPA calculations, taking the random face-centered cubic (fcc) Ti 1âĹŠx Al x (0 âĽď x âĽď 1) alloy as example. For the CPA and SQS calculations, we employ the Exact Muffin-Tin Orbitals (EMTO) method and the pseudopotential method as implemented in the Vienna Ab initio Simulation Package (VASP), respectively. We show that the composition dependences of the VASP-SQS and EMTO-CPA parameters are in good agreement with each other. The energy associated with the LLD increases with x up to x = 0.625 âĹij 0.750 and drops drastically thereafter. The influence of the LLD on the lattice constants, mixing energy, and C 12 elastic constant is negligible. C 11 and C 44 decrease after atomic relaxation for alloys with large LLD, however, the trends of C 11 and C 44 are not significantly affected. In general, the uncertainties associated with the symmetry lowering turn out to be superior to the differences between the two techniques including the effect of LLD.

• guisheng@kth.se