Generalized stacking fault energy of γ-Fe

•***Wei Li*** [1] ***Song Lu*** [1] ***Qing-Miao Hu*** [2] ***Börje Johansson*** [1,3] ***Se Kyun Kwon*** [4]
Mikael Grehk [5] ***Jan Y. Johnsson*** [6] ***Levente Vitos*** [1,3,7]

[1] *Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology, Stockholm SE-100 44, 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] *Graduate Institute of Ferrous Technology, Pohang University of Science and Technology, Pohang 790-784, Korea*
[5] *AB Sandvik Materials Technology, SE-811 81 Sandviken, Sweden*
[6] *Outokumpu Stainless AB, Avesta Research Centre, SE-774 22 Avesta, Sweden*
[7] *Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, H-1525 Budapest, P.O. Box 49, Hungary*

We investigate the generalized stacking fault energy of paramagnetic γ-Fe as a function of temperature. At static conditions, the face centered cubic lattice is unstable with respect to the hexagonal close packed lattice, resulting in negative intrinsic stacking fault energy (ISF) and large positive unstable stacking fault energy (USF). The ISF has a strong positive temperature coefficient, turning positive around 300 K. The USF decreases monotonously with temperature. According to the recent plasticity theory, the overall effect of temperature is to move the system from the stacking fault formation regime ($T \ll 300\,\mathrm{K}$) towards maximum twinning ($T \approx 300\,\mathrm{K}$) and finally to a dominating full-slip regime ($T \gg 300\,\mathrm{K}$).

• wei2@kth.se