Point defect formation entropy on the example of FeO at high temperatures

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Point defects have a significant impact on various properties of solids. The concentration of defects in thermodynamic equilibrium can be described in terms of free energy of formation. Which under the assumption of Arrhenius behavior can be divided into the energy and entropy of defect formation. Quite often the entropy term is neglected as insignificant, but at sufficiently large temperatures in some crystals the contribution can be quite large.

Correct calculation of the entropies of defect formation is a challenging task. Within the framework of the FeO iron oxide model with the Tersoff potential [1], using previously obtained equilibrium concentrations of defects from direct molecular dynamic simulations of the two-phase system, in this work we propose a consistent way to calculate the entropies of formation using thermodynamic integration and taking into account the behavior of the external chemical potential.

The rather strict limitations of thermodynamic integration in the crystal at high temperatures, the impact of the external chemical potential, and the explicit connection between the entropy of formation and vibrational enotropy will be highlighted.

The reported study was funded by RFBR and ROSATOM according to the research project No. 20-21-00159.

[1] Byggmästar J, Nagel M, Albe K, Henriksson K O E and Nordlund K 2019 *Journal of Physics: Condensed Matter* **31** 215401