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Vibrational entropy changes the solid solubility of a random alloy at high temperatures[1] NINA SHULUMBA, Linköping University Sweden, OLLE HELLMAN, California Institute of Technology USA, ZAMAAN RAZA, Linköping University Sweden, JENIFER BARRIRERO, FRANK MÜCKLICH, Saarland University Germany, IGOR A. ABRIKOSOV, MAGNUS ODÉN, Linköping University Sweden — We have developed a method to accurately and efficiently determine vibrational entropy as a function of temperature and volume for substitutional alloys from first principles. Using $Ti_{1-x}Al_xN$ metal alloy as a model system we calculate the isostructural phase diagram by minimization of the free energy, solving the original Gibbs problem of finding its global minimum corresponding to the true equilibrium state of the system. We demonstrate that the vibrational contribution to the free energy has a decisive impact on the calculated phase diagram of $Ti_{1-x}Al_xN$ alloy, lowering the maximum temperature for the miscibility gap from 9000 K to 2400 K. The solubility limit of the predicted phase diagram is experimentally verified by local chemical composition measurements of thermally aged $Ti_{50}Al_{50}N$ alloys.

[1]DocMASE, SECO Tools AB, SSF RMA 08-0069 and SRL 10-002, VR 2012-4401 and 637-2013-7296, Vinnova M-ERA.net, MC2, (KAW) (Isotopic Control for Ultimate Material Properties).

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