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Monte Carlo Calculations of Finite Temperature Transition Rates in Nickel[1] ERIK WELCH, Ohio State University, KADEN HAZZARD, Ohio State University, JOHN WILKINS, Ohio State University — Experiments reveal that self diffusion for many fcc and bcc metals is enhanced at high temperatures, thereby deviating from expected Arrhenius behavior. For nickel it is expected the deviation is caused by the influence of the di-vacancy mechanism in addition to the dominant single vacancy mechanism, but zero temperature *ab initio* calculations suggest this is not the case. We investigate finite temperature effects due to anharmonicity in the potential for the single vacancy mechanism in nickel using a classical EAM potential. We modify the recently developed Wang-Landau Monte Carlo method to extract the vibrational density of states along a continuous spatial reaction coordinate. This allows the calculation of the transition rate within full transition state theory at finite temperature. We find our results agree with the harmonic approximation at low temperature and we compare our high temperature results with experiment.

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