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Short-Range Order Effects on the Thermodynamic Properties of the Ni_3Al Alloy[1] ALEX ANTONELLI, BERNARDO MEIRELLES, Universidade Estadual de Campinas, CAETANO MIRANDA, Massachussetts Institute of Technology — The reasons for the substantial changes induced by disorder in the thermodynamic properties of the Ni_3Al alloy still remain controversial. While several computational studies have found a significant increase in both vibrational entropy and volume as the alloy becomes disordered, there is also evidence that these properties remain unchanged upon disordering. In this work, we present a computational study of the excess vibrational entropy and excess volume of the disordered Ni_3Al alloy, in which, we focused on the interplay between short-range order and long-range order effects on these properties. Using the Simulated Annealing optimization technique, we obtained several structures that exhibit no long- range order, but have different degrees of short-range order. Excess vibrational entropies were computed using an empirical potential, while excess volumes were obtained using both: an empirical potential and *ab initio* techniques. Our calculations indicate that, both excess vibrational entropy and excess volume are substantially reduced in alloys that have no long-range order but have some degree of local order. Both methodologies used to model the alloy give rise to similar results for the excess volume, indicating that the short-range effects are not an artifact of how the system is modelled.

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Alex Antonelli
Universidade Estadual de Campinas

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