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Temperature specification in atomistic molecular dynamics and its impact on simulation efficacy

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Abstract content
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The importance of temperature as an energy related state function in physical systems was well established from the earliest days of the physical sciences and was central to the formulation of the laws of thermodynamics. These laws fundamentally state that for an isolated system, knowledge of temperature leads to an assessment of system entropy, which in a sense conveys the stability of the system above absolute zero temperatures. As the development of theoretical and computational methods continues rapidly in diverse branches such as chemistry, condensed matter physics, material science, molecular biology, nanotechnology and others, the effect of temperature on the simulated parameters remains at the heart of all problems. This paper discusses the currently used temperature modelling formalisms in atomistic molecular dynamics simulations. Standalone simulation programs may have variability in the definition of temperature and its evolution in a system. For instance, some specifications of temperature are done indirectly in terms of its effect on the elongation of the lattice parameters, while others employ energy equi-partition and thermostatic approaches. In heuristic simulation programs which are essentially closed off from dissection, this question does not really arise directly but inherently where specification of temperature occurs in the form of a single, external input variable. Simulation as a means of materials research is projected to grow in popularity due to vastly improved computational power and a diversity of research questions for which no commercial programs exist per se. Therefore, standalone programs are also likely to grow in prominence, necessitating clarification of temperature specification. Therefore, we attempt to address the fundamental question of optimal temperature specification in the context of atomistic molecular dynamics simulation context. In particular, we calculate the vacancy formation energies for a number of FCC metals using two separate temperature specification approaches and then discuss the results.

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