Finite temperature Cauchy-Born approximation for System with Dilute Defects

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Constitutive relations play important roles in the study of particular materials. Either experiments or massive simulations were needed to get such material properties. In this talk, I will introduce our recent work on the efforts of effectively evaluating material constitutive relations. It can be considered as generalization of traditional Cauchy-Born approximation, which only works for perfect system at zero-temperature.

References:

[1] J. L. Ericksen, On the Cauchy-Born rule, Mathematics and Mechanics of Solids, 13, 199-220(2008).

[2] Jerry Z. Yang, Chao Mao, Xiantao Li, and Chun Liu, On the Cauchy–Born approximation at finite temperature, *Computational Materials Science,* 99, 21-28 (2015).