

On the Cauchy-Born Approximation at Finite Temperature

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We address several issues regarding the derivation and implementation of the Cauchy-Born approximation of the stress at finite temperature. In particular, an asymptotic expansion is employed to derive a closed form expression for the Piola-Kirchhoff stress. The derivation takes into account the translational invariance and clarifies the removal of the zero phonon modes. Also revealed by the asymptotic approach is the role of the smoothness of the interatomic potential. Several numerical examples are provided to validate this approach.