

Thermo-coupled Surface Cauchy-Born Theory: An Engineering Finite Element Approach to Modeling of Nanowire Thermomechanical Response - DTU Orbit (08/11/2017)

Thermo-coupled Surface Cauchy-Born Theory: An Engineering Finite Element Approach to Modeling of Nanowire Thermomechanical Response

There are remarkable studies geared towards developing thermomechanical analyses of nanowires based on quasiharmonic and Molecular Dynamics simulations. These methods exhibit limited applicability due to the associated computational cost. In this study an engineering finite-temperature model based on Surface Cauchy-Born theory is developed, where surface energy is accounted for in the prediction of the thermomechanical response. This is achieved by using a temperature-dependent interatomic potential in the standard Cauchy-Born theory with a surface energy contribution. Simultaneous calculation of thermal and mechanical stresses is achieved by eliminating the diagonalization matrix of entropy in the quasiharmonic system. This leads to a reduction in the degrees of freedom by more than 99% in comparison with equivalent Molecular Dynamics models. For the purpose of validation, results obtained on copper and nickel nanowires through the proposed method are compared with those of the more involved Molecular Dynamics simulations. This comparison verifies the significant reduction in the computational process with an acceptable accuracy. Hence, the proposed method provides a promising engineering tool without compromising the underlying physics of the problem and has potential implications in the effective modeling of the nanoscale thermomechanical behavior.

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Authors: Esfahania, M. N. (Ekstern), Sonne, M. R. (Intern), Hattel, J. H. (Intern), Alaca, B. E. (Ekstern)

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