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Energy-based Approach to Limit States in Nanostructures. Calculation of the Critical Values of Energy from Firt Principles

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The application of the energy-based approach to limit states proposed by Rychlewski for elastic materials can appear helpful in the field of nanomechanics filling the gap between atomistic calculations and continuum mechanics modelling of the behaviour of different kinds of crystalline nanostructures. We propose to calculate the critical energy of pertinent proper elastic states from quantum mechanical theory of nanostructures. The quantum mechanical model for an ideal single crystal of Cu is studied and the comparison with the results obtained for Al crystal is made. Using the Wigner–Seitz cellular approach and the Slater method the structure of the s, d, f and p energy bands was calculated. This enables obtaining of the internal energy of the crystal volume confined in the deforming Wigner-Seitz cell. Finally the critical energy for the particular proper state was determined.

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