Thermomechanical Continuum Representation of Atomistic Deformation at Arbitrary Time and Size Scales

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A thermomechanical equivalent continuum (TMEC) theory for the deformation of atomistic particle systems at arbitrary size and time scales has recently been developed. The description of coupled thermomechanical continuum behavior is derived directly "from the ground up", using molecular dynamics concepts. This theory is a further advancement from a pure mechanical equivalent continuum (EC) theory developed recently. These new theories provide fully dynamic continuum interpretations of atomistic deformation with different resolutions for atomic particle motion. While the mechanical theory is based on an explicit and full resolution of the atomistic motion, the thermomechanical theory is based on a decomposition of the atomic particle velocity into a relatively slower-varying structural deformation part and a high-frequency thermal oscillation part. Within the meaning of classical mechanics, the TMEC theory establishes the ultimate atomic origin of coupled thermomechanical deformation phenomena at the continuum level. Because the decomposition of atomic velocity into a structural deformation part and a thermal oscillation part is intrinsically dependent on both size- and time-scales and because the theory is explicitly formulated for an arbitrary size scale, the development allows scale-sensitive characterizations of both structural deformation and heat conduction. On one hand, balance of momentum at the structural level yields fields of stress, body force, traction, mass density and deformation as they appear to a macroscopic observer. The full dynamic equivalence between the discrete system and continuum system includes (i) preservation of linear and angular momenta, (ii) conservation of internal, external, and inertial work rates, and (iii) conservation of mass. On the other hand, balance of momentum for the thermal motions as it appears to an observer moving at the structural velocity yields the fields of heat flux and temperature. These quantities can be cast in a manner as to conform to the continuum phenomenological equation for heat conduction and generation, yielding scale-sensitive characterizations of specific heat, thermal conductivity, and thermal relaxation time. The coupling between the structural deformation and the thermal conduction processes results from the fact that the equations for structural deformation and for heat conduction are two different forms of the same balance of momentum equation at the fully time-resolved atomic level. This coupling occurs through an inertial force term in each of the two equations induced by the other process. For the structural deformation equation, the inertial force term induced by thermal oscillations of atoms gives rise to the phenomenological dependence of deformation on temperature. For the heat equation, the inertial force term induced by structural deformation takes the phenomenological form of a heat source.