A New Equation for Period Vectors of Crystals under External Stress and Temperature in Statistical Physics

Mechanical Equilibrium Condition and Equation of State

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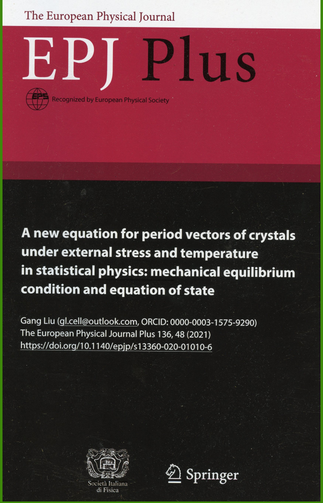
Abstract

Starting with the rigorous derivation of the work done on the center cell by external forces, a new equation is derived for the period vectors (cell edge vectors) in crystals under external stress and temperature. Since the equation is based on the principles of statistical physics, it applies to both classical and quantum systems. The existing theory for crystals under external pressure is covered as a special case. The new equation turns out to be the mechanical equilibrium condition and the equation of state for crystals under external stress and temperature. It may be used to predict crystal structures and to study structural phase transitions and crystal expansions. For linear elastic crystals, it takes the microscopic and temperature-dependent form of the generalized Hooke's law, and may therefore be used to



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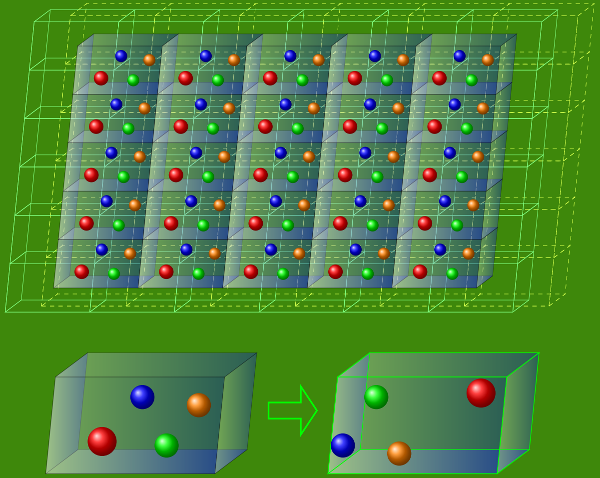
The work done on the center cell by the external stress $\mathbf{S}$

$$dW = (\mathbf{S}\cdot\sigma_{\mathbf{a}})\cdot d\mathbf{a} + (\mathbf{S}\cdot\sigma_{\mathbf{b}})\cdot d\mathbf{b} + (\mathbf{S}\cdot\sigma_{\mathbf{c}})\cdot d\mathbf{c} \tag{1}$$



Then based on the principles of statistical physics, the new equation determining the period vectors $(\mathbf{a}, \mathbf{b}, \mathbf{c})$ for crystals under external stress $\mathbf{S}$ and temperature T:

$$\mathbf{S} \cdot \sigma_{\mathbf{h}} = -\frac{1}{\beta} \frac{\partial \ln Z}{\partial \mathbf{h}} \quad (\mathbf{h} = \mathbf{a}, \mathbf{b}, \mathbf{c}), \tag{2}$$

where $\beta = 1/(kT)$, and k and Z are the Boltzmann constant and the system partition function. The cell surface vectors are $\sigma_{\mathbf{a}} = \mathbf{b} \times \mathbf{c}$, $\sigma_{\mathbf{b}} = \mathbf{c} \times \mathbf{a}$, and $\sigma_{\mathbf{c}} = \mathbf{a} \times \mathbf{b}$.

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The net force by the left half on the right half of the one-dimensional crystal

$$F_{L\to R}(a) = -\frac{d}{da}E_p^{(L-J)}(a) \tag{3}$$

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$$= \sum_{j=1}^{\infty}\frac{4\epsilon}{a}\left[12\left(\frac{\lambda}{ja}\right)^{12}-6\left(\frac{\lambda}{ja}\right)^{6}\right] \tag{5}$$