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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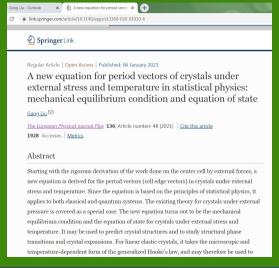
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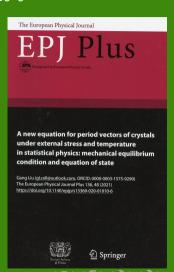
The derived equation

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2 The derived equation

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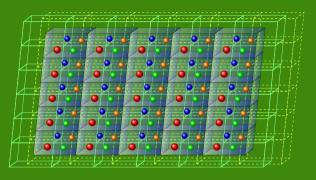


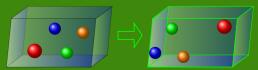
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The derived equation

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

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

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

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

$$= \frac{1}{2} \sum_{j=-\infty}^{\infty(j\neq 0)} j f^{(L-J)}(ja)$$
(4)

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