Dmitriev *et al.* Reply: In their Comment, Horowitz, Gooding, and Krumhansl[1] (HGK) propose that for reconstructive transitions in which large-scale displacements of the atoms take place, the dependence of the equilibrium order parameter η on the average atomic displacements ξ, which was introduced empirically in our Letter,[2] should be related to a density-wave expansion of the lattice. This suggestion is interesting and fruitful, but, in our opinion, should be complemented by the following clarifying remarks.

(1) The more essential property of $\eta(\xi)$ is that it be a *transcendental periodic function in some symmetric direction of the lattice*, along which the symmetry of the system is *increased* for specific displacements. In all the other directions, η is only a *nonlinear aperiodic* function of ξ. This property was illustrated by the various examples discussed in our Letter[2] (see also Ref. 3) and is confirmed by the expression of $\rho(x)$ found by HGK for the β-ω transition [Eq. (1) of Ref. 1]. Let us show that for the additional example of a square-to-triangular lattice, introduced by HGK in their Comment, one also gets a transcendental periodic dependence for $\eta(\xi)$.

It is well known that there are many crystallographic paths which reach a triangular lattice (space group $P6mm$) from a tetragonal ($P4mm$) lattice. In the path chosen by HGK the $P6mm$ symmetry can be obtained when two independent sets of shifts take place along the x and y axes. These *symmetric* shifts are

$$x = R_0, 2R_0, 3R_0, \ldots, \qquad y = 2R_0(1-\sqrt{3}/2), 4R_0(1-\sqrt{3}/2), \ldots, \tag{1}$$

where R_0 represents the atomic radius and is connected with the lattice parameters of the tetragonal (a_T) and triangular (a_h) unit cells by $R_0 = \frac{1}{2} a_T = \frac{1}{2} a_h$. Accordingly, we deal with a two-component order parameter, where the two components can be written

$$\eta_1 = \eta_0 \sin\left(\frac{\pi}{R_0} x\right), \quad \eta_2 = \eta_0 \sin\left(\frac{\pi}{R_0} y\right), \tag{2}$$

where η_0 is the amplitude of the displacement.

Let us note that for a general nonsymmetric displacement along x or y, the symmetry of the tetragonal lattice is lowered to monoclinic ($P2$), and increases to orthorhombic ($P2ma$) for the symmetric shifts x (or y) equal to $R_0, 2R_0, 3R_0$. When the symmetric shifting given by (1) occurs simultaneously along the two axes x *and* y, the hexagonal $P6mm$ symmetry is obtained.

The thermodynamic potential of the reconstructive $P4mm \rightarrow P6mm$ transition has the form

$$F = a_1(\eta_1^2+\eta_2^2) + a_2(\eta_1^4+\eta_2^4) + a_3\eta_1^2\eta_2^2 + b(\eta_1^2-\eta_2^2)(e_{xx}-e_{yy}) + c_{12}(e_{xx}-e_{yy})^2,$$

in which the combination of strain-tensor components $(e_{xx}-e_{yy})$ appears as an induced secondary order parameter. Thus, the transition can be characterized as an *improper ferroelastic transition* associated with the wave vector $q=0$.

A thermodynamically more advantageous path may be proposed, corresponding to the wave vector $q = \frac{1}{2} a_T^*$. The symmetric displacements in this case are $x = R_0/2$, $R_0, 3R_0/2, \ldots$ and $y = R_0(1-\sqrt{3}/2), 2R_0(1-\sqrt{3}/2), \ldots$. When an arbitrary nonsymmetric shifting occurs along only one direction (x or y), the symmetry becomes orthorhombic $P2bm$.

(2) Following Alexander and McTague,[4] HGK assume that only the Fourier coefficients $\rho(q)$ with smallest q are to be considered. We disagree with this assumption, as it is clear that the relevant transition wave vectors are actually determined by the size of the atoms, i.e., $q = \pi/R_0$, and thus one should also take into account coefficients $\rho(q)$ with finite (not small) values of q.

(3) In the Comment, no actual connection between our phenomenological approach and microscopic theories is given. Although we do not have a general solution for this problem, we have shown[5] that for a three-level system (for example, a unit cell with three ordered positions), one can find explicitly the form of the order parameter as a transcendental function of the microscopic probability of occupation levels.

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