Two-dimensional mixed crystals

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We show that the long-range positional order in a two-dimensional crystal \( A_1 \ldots B_x \) is destroyed by size-mismatch disorder. The size-mismatch disorder is characterized by an effective temperature \( k_B T_D = K x (1-x) (L_B^0 - L_A^0)^2 \) associated with the strain energy, where \( K \) is a force constant and \( L_B^0 - L_A^0 \) is the length mismatch. We study a model that has a fixed triangular-net topology. By comparison with computer simulations, we show that a linearized small displacement theory is adequate for small size mismatches. The long-range orientational order remains. The positional correlation function decays algebraically, which leads to power-law peaks that replace the Bragg peaks in the diffraction pattern. We argue that this model should provide a reasonable qualitative description of real two-dimensional mixed crystals, in the limit of a small size mismatch.

I. INTRODUCTION

The melting transition has been extensively studied in single component two-dimensional systems.\(^1\)\(^-\)\(^3\) It is known that thermal fluctuations destroy the long-range positional order at any finite temperature. This produces a phase with quasi-long-range-order that is characterized by a power-law decay in the position-position correlation function at all temperatures up to some temperature \( T_1 \). This phase has power-law peaks in the diffraction pattern, where the Bragg peaks would have been. However, the long-range orientational order remains all the way up to \( T_1 \) above which the angular correlations decay algebraically, in the \textit{hexatic} phase.\(^5\) Finally at some higher temperature \( T_2 \), melting is completed, and both the positional and angular correlations fall off exponentially. At this time the evidence is inconclusive as to whether \( T_2 \) is higher than \( T_1 \) or whether \( T_1 \) and \( T_2 \) are coincident.

In this paper we investigate the idea that the size mismatch between the two components in a two-dimensional random alloy \( A_1 \ldots B_x \) also destroys the long-range positional order in an analogous way to the thermal disorder in a single component system, as previously discussed by Nelson.\(^5\) We set up a triangular network with nearest neighbor forces with spring constant \( K \) and natural spring lengths \( L_A^0 \) and \( L_B^0 \). The topology of this network cannot be changed and every atom always has the same six nearest neighbors so that the disorder is quenched in. Nevertheless, the long-range positional order is destroyed, even though the fixed topology prohibits the formation of either \textit{disclinations} or dislocations.\(^5\) Our approach is analogous to the spin wave description of the thermal disordering of the classical \( XY \) model.\(^6\)\(^,\)\(^7\)

We show that it is possible to define an effective temperature \( T_D \) associated with the disorder via

\[
k_B T_D = K x (1-x) (L_B^0 - L_A^0)^2 ,
\]

where \( L_B^0 - L_A^0 \) is the length mismatch. The triangular lattice is shown in Figs. 1 and 2, with two kinds of bonds \( A \) and \( B \) that are randomly located in the lattice with probabilities \( 1-x \) and \( x \), respectively. This mathematical simplification to \textit{bond} disorder rather than \textit{site} disorder does not qualitatively affect any of our results. For example, if the lattice is made up of randomly positioned \( A \) and \( B \) sites with probabilities \( 1-x \) and \( x \), respectively, then the disorder temperature in Eq. (1) is replaced by

\[
k_B T_D = \frac{1}{2} K x (1-x) (L_B^{01} - L_A^0)^2 ,
\]

where \( L_A^{00} \) and \( L_B^{01} \) are the lengths of the \( AA \) and \( BB \) bonds, and the \( AB \) bonds have natural lengths \( L_{AB}^0 = \frac{1}{3}(L_B^{01} + L_A^0) \).\(^8\) Other models for the length disorder would lead to more complex expressions for \( T_D \).

In the next section we recall that the short-range properties are entirely conventional and similar to those in higher dimensions. In Sec. III, we show that the decay of the positional correlations is controlled by the parameter \( \eta \), which leads to power-law peaks in the diffraction pattern if \( \eta < 2 \). In Sec. IV it is shown that the angular correlations do display long-range order which is calculated. Throughout this paper we compare our results with computer simulations. In Secs. III and IV, we show that the positional order is finally destroyed when the lattice \textit{pleats}.\(^9\) The pleating is not described by our linear-

FIG. 1. The regular triangular lattice.
FIG. 2. The relaxed triangular lattice with two different kinds of bonds with different natural lengths. The concentration $x = 0.5$; the shorter bonds are shown as dashed lines, and the longer bonds as solid lines. The length-mismatch parameter $\langle L_B^0 - L_A^0 \rangle / \langle L \rangle$ is 30%.

ized approach, and is brought about by the fixed topology that prevents a more reasonable disordering of the lattice at a smaller length mismatch. Nevertheless, the pleating is of some interest in its own right as it relates to the crumpling transition; the difference being that no motion out of the plane is permitted in pleating whereas it is permitted in crumpling. We stress that the pleating transition is unphysical, because of the absence of any repulsive forces at short distances in our model, as well as the imposition of a fixed topology. The pleating transition takes place at a length mismatch of about 50% which is way beyond the region of physical interest as no random solid solutions can tolerate length mismatches of more than about 15%. In Sec. V we discuss finite-size scaling and in the Conclusions, we explore ways in which the model needs to be modified to give a more realistic description of size-mismatch effects in two dimensions.

II. SHORT-RANGE PROPERTIES

The triangular network is described by a potential

$$V = \frac{K}{2} \sum_{ij} (L_{ij} - L_{ij}^0)^2,$$

where $K$ is the force constant between nearest neighbor atoms, denoted in the summation by the angular brackets. The length of the bond $ij$ in the network is $L_{ij}$ and the natural (unstrained) length of this bond is $L_{ij}^0$. The bonds are chosen randomly on a triangular network to be either type $A$ with probability $1-x$ or type $B$ with probability $x$.

The short-range properties of this model have been well studied and are qualitatively the same in two and three dimensions, as summarized below. The network is relaxed so as to minimize the strain energy. This gives fairly broad distributions of the $A$ and $B$ bond lengths, from which the mean lengths are given by,

$$\langle L_A \rangle = L_A^0 + \frac{x}{3}(L_B^0 - L_A^0),$$
$$\langle L_B \rangle = L_B^0 - \frac{1-x}{3}(L_B^0 - L_A^0),$$

where the angular brackets $\langle \cdots \rangle$ denote an ensemble average. The mean overall length, which determines the size of the sample obeys Vegard's law\cite{13}

$$\langle L \rangle \equiv (1-x)\langle L_A \rangle + x\langle L_B \rangle = (1-x)L_A^0 + xL_B^0.$$ (5)

The widths of the $A$ and $B$ distributions are equal and given by

$$\langle L_A^2 \rangle - \langle L_A \rangle^2 = \langle L_B^2 \rangle - \langle L_B \rangle^2 = \frac{2}{3}x(1-x)(L_B^0 - L_A^0)^2.$$ (6)

The total strain energy $E_s$ can also be found, and is given by

$$\frac{E_s}{N} = \frac{1}{2}Kx(1-x)(L_B^0 - L_A^0)^2 = \frac{1}{2}k_B T_D,$$ (7)

where $N$ is the number of sites and the disorder temperature $T_D$ has been previously defined in Eq. (1).

III. DIFFRACTION PATTERN

In three dimensions, the model (3) on say a face-centered-cubic lattice, leads to conventional Bragg peaks and associated Huang scattering in the diffraction pattern. The situation is very different in two dimensions. Assuming the scattering length of all atoms to be unity, the elastic scattering cross section for neutrons can be written as

$$I(Q) = \frac{1}{N} \sum_{ij} e^{iQ \cdot \mathbf{r}_0} e^{iQ \cdot \mathbf{u}_{ij}}.$$ (8)

where $Q$ is the momentum transfer. In this equation, $\mathbf{r}_0$ is the equilibrium position of atom $i$, and the average displacement $\langle \mathbf{u}_i \rangle$ is required to be zero to define a reference lattice with nearest neighbor distance $a = \langle L \rangle$ as given by Eq. (5). The approximation for the average needed to evaluate (8), up to terms $O(Q^4)$ is

$$\langle e^{iQ \cdot \mathbf{u}_i} \rangle = C_Q(R) \approx e^{-\frac{1}{2}(\langle Q \cdot Q \rangle)}.$$ (9)

This is defined as the density-density correlation function $C_Q(R)$, where $R$ is distance between sites $i$ and $j$. From our previous work\cite{15}

$$\langle \mathbf{u}_i \cdot \mathbf{u}_j \rangle = -Kx(1-x)(L_B^0 - L_A^0)^2 G_{ij}$$ (10)

which is similar to the relationship for long wavelength phonons in a single component lattice at a temperature $T$, if we were to replace $Kx(1-x)(L_B^0 - L_A^0)^2$ by $k_B T$. Using (10) we have

$$\mathbf{Q} \cdot (\mathbf{u}_i \cdot \mathbf{u}_j) \approx -\frac{K}{2}x(1-x)(L_A^0 - L_B^0)^2 [\mathbf{Q} \cdot (\mathbf{G}_{ii} + \mathbf{G}_{jj} - 2\mathbf{G}_{ij}) \cdot \mathbf{Q}].$$ (11)
The Green's function can be written in \( k \) space using the Fourier transform
\[
G_{ij} + G_{ji} - 2G_{ij} = \frac{2}{N} \sum_k \mathbf{G}(k)(1 - e^{i \mathbf{k} \cdot \mathbf{R}^0_{ij}}). \tag{12}
\]

For small \( k \) we may write
\[
\mathbf{G}(k) = \frac{A_L \mathbf{k} + A_T (1 - \mathbf{k})}{k^2}, \tag{13}
\]
where, for the triangular lattice,\(^{16}\)
\[
A_T = 3A_L = \frac{8}{3a^2K} \tag{14}
\]
and \( a = \langle L \rangle \) is the lattice constant. Evaluating the integrals we have
\[
\frac{1}{4}(Q \cdot u_{ij})^2 = Kx (1-x)[Q(L^0_B - L^0_A)]^2 \sum_k \frac{A_T + (A_L - A_T)(\hat{Q} \cdot \mathbf{k})^2}{k^2}(1 - e^{i \mathbf{k} \cdot \mathbf{R}^0_{ij}}) \tag{15}
\]
\[
= Kx (1-x)[Q(L^0_B - L^0_A)]^2 \frac{\sqrt{3}a^2}{8\pi}(A_L + A_T)\ln R^0_{ij} + \text{const},
\]
where we have used the integral,
\[
\int \frac{1 - e^{i \mathbf{k} \cdot \mathbf{R}^0_{ij}}}{k^2} \, d^2k = 2\pi \ln R^0_{ij} + \text{const}, \tag{16}
\]
which is valid for large \( R^0_{ij} \). The logarithmic distance dependence in (16) comes from the integrand around the origin, where the approximation (13) is valid. This leads us to the result
\[
e^{-\frac{1}{2}(Q \cdot u_{ij})^2} = \frac{B(Q)}{(R^0_{ij})^\eta} \tag{17}
\]
and hence
\[
C_Q(R) = \frac{B(Q)}{R^\eta}, \tag{18}
\]
where to leading order we can ignore the difference between \( R^0_{ij} \) and \( R \). The exponent \( \eta \) given by
\[
\eta = Kx (1-x)[Q(L^0_B - L^0_A)]^2 \frac{\sqrt{3}a^2}{8\pi}(A_L + A_T)
\]
\[
= \frac{4}{3\sqrt{3}\pi}x (1-x)[Q(L^0_B - L^0_A)]^2. \tag{19}
\]
The correlation function \( C_Q(R) \) has the same form as that derived by Nelson,\(^5\) with Lamé constants \( \lambda = \mu = \sqrt{3}K/4 \) and the real temperature replaced by \( T_D \) from Eq. (1), plotted in Fig. 3. The results are averaged over the six equivalent nearest neighbor bond directions. Both the longitudinal and transverse distortions contribute to \( \eta \) in (19) through \( A_L \) and \( A_T \). A similar result to Eq. (19) for site rather than bond disorder leads to a result for \( T_D \) as given in Eq. (2). In the site case, the distortions around each site have radial symmetry, which means that only the long wavelength \( \text{longitudinal} \) distortions contribute to \( \eta \) through \( A_L \).\(^8\) The algebraic decay of the correlation function (18) is checked against computer simulations as shown in Fig. 3, where the amplitude \( B(Q) \) is treated as an adjustable constant. We can see that the theoretical approximation (18) is adequate.

The disordering of the perfect lattice is controlled by the parameter \( \eta \) which is determined by the size mismatch rather than the temperature.\(^5\) From the result (18), we are able to calculate the asymptotic form of the \( I(q) \) around the reciprocal lattice vector at \( q = Q - q \), where \( q \) is measured from the nearest reciprocal lattice vector \( g \). Divergent behavior is found for peaks with \( \eta < 2 \). Combining Eqs. (8), (9), and (18), we have
\[
I(q) = \int_q^\infty \int_0^{2\pi} e^{i q R \cos \theta} \left( \frac{a}{R} \right)^\eta R \, dR \, d\theta
\]
\[
= \int_q^\infty J_0(q R) \left( \frac{a}{R} \right)^\eta R \, dR
\]
\[
= a^\eta R^{-2} \int_q^\infty J_0(\alpha x^\frac{1}{2} - \eta) \, dx. \tag{20}
\]

**FIG. 3.** The density-density correlation function \( C_Q(R) \) plotted against the distance \( R \) in units where the mean bond length is unity. The results are averaged over the six equivalent nearest neighbor bond directions. The length-mismatch parameter \( (L^0_B - L^0_A)/(L) \) is 4% and the results are averaged over four samples, each of which is 100x100. The solid line is using the theory in Eqs. (18) and (19) where the amplitude \( B(Q) \) is treated as an adjustable parameter. The upper line is for \( Q_1a = 3\pi \) and the lower curve for \( Q_2a = 4\pi \); neither of which are reciprocal lattice points.
When $\eta < 2$, the kernel of the integral is well behaved at the low cut off which can be replaced by zero. The integral (20) contributes a multiplier and $I(q)$ is divergent at small $q$ as $q^{-(2-\eta)}$ where $q$ is measured from the reciprocal lattice vector. For $\eta > 2$, there is no divergence, but an upward-pointing cusp that goes as $q^{\eta-2}$ should exist for $2 < \eta < 3$. We find no evidence for such a cusp in Fig. 4 so that the cusp amplitude must be small. For $\eta > 3$, $I(q)$ and its derivative are continuous. There is no limit of any peaks around the reciprocal-lattice vectors in Fig. 4 when $\eta > 2$.

The pleating transition occurs at a length mismatch of about 50%, so that the pleating is very apparent at a length mismatch of 60% as shown in Fig. 5. Just before a 50% length mismatch, a few sites begin to pleat and the number increases rapidly as the size mismatch exceeds 50% as shown in Fig. 6. A pleated site is defined to have all six bonds to its nearest neighbors lying to one side within the 180° arc of a semicircle. The network chooses this form of disordering for large size mismatches because it is prevented from forming dislocations and disclinations as occurs in the thermal case. In the thermal case, the solid begins to melt as first dislocations and then disclinations begin to unbind, destroying the topological order. However, the topology is preserved in our model even when pleating occurs because the six nearest neighbors of a site remain fixed.

IV. ANGULAR CORRELATIONS

Long-range angular correlations are present and can be calculated within our model. The angular correlation function is defined as

$$C_{\phi}(R) \equiv \left| \langle e^{i\phi_{ij}} \rangle \right|,$$

where $\theta_{ij} = \theta_i - \theta_j$ is the angle between two bonds emanating from lattice points $i$ and $j$, and $R$ is their separation. It is convenient to measure the $\theta_{ij}$ from the underlying reference lattice, but it could also be measured from the line joining the sites $i$ and $j$; the result would be the same to leading order. Because long-range angular correlations exist, for large $R$,

$$\langle e^{i\phi_{ij}} \rangle \rightarrow \langle e^{i\theta_{ij}} \rangle \langle e^{-i\theta_{ij}} \rangle,$$

and

FIG. 4. The lower panel shows the diffracted intensity $I(Q)$ plotted against the momentum variable $Q_x$, where the $x$ direction contains a nearest neighbor bond, and the results are averaged over the six equivalent directions. The length-mismatch parameter $(L_B^2 - L_A^2)/\langle L \rangle$ is 4% and an average is taken over 87 samples of $40 \times 40$ triangular lattices. The upper panel shows the diffracted intensity around the reciprocal lattice points in the lower panel but in the perpendicular direction. The dashed lines are for guidance of the eye.

FIG. 5. The relaxed triangular lattice after pleating has occurred. The length-mismatch parameter $(L_B^2 - L_A^2)/\langle L \rangle$ is about 60%.

FIG. 6. Showing the long-range angular correlation $C_{\phi}(\infty)$, the pleating $P$, and the microscopic and macroscopic lengths $\langle L \rangle$ plotted against the length-mismatch parameter $(L_B^2 - L_A^2)/\langle L \rangle$. The symbols are from the computer simulations and the dashed and solid lines are the theoretical results from (31) and (5).
\( e^{-\theta_6} = |e^{-i\theta_6}| = e^{-\left(1/2\right)(i\theta_6)^2} \)  

(23)

and only the deviation \( \delta \theta = \theta - n \pi/3 \), where \( n \) is integer, is needed.

\[
W_6 = \frac{18(u_{12}^2 - (u_{12} \cdot R_{12}^0)^2)}{\langle L \rangle^2} = -36Kx(1-x) \left[ \frac{(L_0^0 - L_B^0)}{\langle L \rangle} \right]^2 \text{Tr}[(1-R_{12}^0 R_{12}^0)(G_{11} - G_{12})],
\]

where we have used Eq. (10). We know that \( R_{12}^0 \cdot (G_{11} - G_{12}) \cdot R_{12}^0 = -d/z \), where \( d \) is the dimension and \( z \) the coordination number.\(^{17}\) For the triangular lattice, \( d/z = \frac{3}{4} \), so that

\[
W_6 = -36Kx(1-x) \left[ \frac{(L_0^0 - L_B^0)}{\langle L \rangle} \right]^2 \text{Tr}[(1-R_{12}^0 R_{12}^0)(G_{11} - G_{12})] - \frac{1}{3}, \tag{26}
\]

where

\[
\text{Tr}(G_{11} - G_{12}) = \frac{1}{N} \sum_k \text{Tr} G(k)(1-e^{iR_{12}^0 / \omega_k})
\]

\[
= \frac{1}{N} \sum_k \text{Tr} G(k)(1-\gamma_k)
\]

\[
= -\frac{1}{N} \sum_k \left[ \frac{1}{\omega_1^2(k)} + \frac{1}{\omega_2^2(k)} \right] (1-\gamma_k) \tag{27}
\]

and \( \omega_1 = \pm \sqrt{D_2} \). The expressions needed are

\[
\gamma(k) = \frac{1}{2}\left( \cos 2x + 2 \cos x \cos y \right), \tag{28}
\]

\[
D_1 = 3 - 2 \cos 2x - 2 \cos x \cos y, \tag{29}
\]

\[
D_2 = (\cos x \cos y - \cos 2x)^2 + 3 \sin^2 x \sin^2 y, \tag{30}
\]

\[
C_\theta(R) = e^{-2W_6}. \tag{32}
\]

where \( x = k_a a/2 \) and \( y = \sqrt{3} k_a a/2 \). The \( k \) integration in (27) is done numerically to give

\[
W_6 = \frac{17.2x(1-x)}{\langle L \rangle} \left[ \frac{(L_0^0 - L_B^0)}{\langle L \rangle} \right]^2 \tag{31}
\]

and for large \( R \) leads to

\[
C_\theta(\infty) = e^{-2W_6}. \tag{32}
\]

The result (32) shows that the long-range angular order always exists in our linearized calculation. When pleating occurs, the long-range angular correlation is destroyed as shown in Fig. 6. We have performed simulations for different length mismatches and the results are shown in Figs. 6 and 7. When there is no pleating, our analytic results agree well with the computer simulations. When pleating occurs, the computer result begins to drop below the prediction. The top panel in Fig. 6 shows a comparison between the calculated long-range angular correlation \( C_\theta(\infty) = \exp(-2W_6) \) and the simulation results. The agreement is very good up to about a 30% length mismatch, when effects due to pleating start to have an effect. The theory predicts that the long-range angular correlations are always present as no account is taken of pleating. In the second panel of Fig. 6 we show the fraction of sites \( P \) that are pleated. This gives the clearest signature of the phase transition, although there is rounding as a result of finite-size effects. The fraction of pleated sites may be thought of as a disordering parameter. In the bottom panel of Fig. 6 we show the microscopic length and the macroscopic length from simulations. The microscopic length, defined as the average bond length, is constant as predicted by the theory (5), while the macroscopic length, deduced from the sample size, decreases above the pleating transition as would be expected. In pleating, the network folds over on itself, in the same manner as a pleat put in a piece of material, and hence reduces the area.

V. FINITE-SIZE SCALING

Because of finite-size effects, the Bragg peaks are never completely eliminated in our simulations. This is because of the artificial long-range order imposed by the periodic boundary conditions. Nevertheless it is convenient to keep these boundary conditions as then every atom has exactly six nearest neighbors. We need to estimate the magnitude of this effect and try to extract the infinite-size behavior from the finite-size simulations. This is easy for some quantities, like \( C_\theta(R) \), and very difficult for others,

FIG. 7. The angular correlation function \( C_\theta(R) \) plotted against \( R \) in units where the mean bond length is unity. The results are averaged over the six equivalent directions defined by the nearest-neighbor bonds. The results were obtained by averaging over nine samples each of which was 40 x 40. The solid line is the asymptotic theory and the various values of the length-mismatch parameter \( (L_0^0 - L_B^0)/\langle L \rangle \) are indicated.
like $I(Q)$. The scattering at the Bragg momentum $g$ is,
from Eqs. (8) and (17).

$$ I(g) = \frac{1}{N} \sum_{ij} \frac{B(g)}{(R^*)^\eta} \propto \int_a^\infty \frac{d^3R}{R^\eta}. $$(33)

For $\eta < 2$ and $L >> a$, this leads to

$$ I(g) \propto L^{2-\eta} $$

and because $L^2 \propto N$, we may write

$$ I(g) \propto L^{-\eta}. $$

(35)

This remnant Bragg peak contains an extra factor $N$ because
it is a Kronecker $\delta$ rather than a Dirac $\delta$ function.\textsuperscript{12} Otherwise the Bragg peaks vanish as the system
gets larger according to Eq. (35). This finite-size scaling law can be verified by computer simulation and we have
roughly verified that it does work using rather small samples
with $L \leq 200$. The Bragg peak of the perfect lattice
($\eta = 0$) has a height proportional to $N$. As disordering is
introduced by increasing $T_D$, and hence $\eta$, this weight is
redistributed locally. In three dimensions, it becomes the
Huang scattering,\textsuperscript{12} while in two dimensions it either becomes
a power-law peak if $\eta < 2$ as shown in Fig. 4. For
large $Q$, the scattering tends to unity as the phases in Eq.
(8) become random. Note that there is always a Bragg
peak at the origin with weight $N$ that represents a Dirac $\delta$ function with weight unity. When $L^{-\eta} \ll 1$, the
scattering profile approaches that of the infinite sample.
In Fig. 4 the Bragg residue contains 30% of the weight of
the first peak, while the second peak has only a 0.75% Bragg residue and is therefore representative of an infinite sample.

VI. CONCLUSIONS

We have shown that the long-ranged properties of a
two-dimensional mixed crystal can be described by a
linearized small displacement theory, as long as the
topology is kept fixed and no disclinations and/or
dislocations are allowed. This is achieved naturally in a spring model with a fixed triangular network topology. While there is always a long-range orientational order present, the

positional correlation function falls off algebraically, leading
to power-law peaks in the diffraction pattern.

This situation is similar to the thermal disordering of
two-dimensional lattices, and indeed many of our results
can be understood if the temperature $T$ in the thermal
case is replaced by the disorder temperature $T_D$ as
defined by the strain energy in Eq. (1) or (2). This model
can be regarded as the analogue of the quadratic $\theta^2$ mod-
el of Zittartz\textsuperscript{6} and Josié et al.\textsuperscript{1} for spin-wave excitations
in the classical $XY$ model in two dimensions. Like our
model, the $\theta^2$ model does not appear to contain any
disclinations or dislocation type excitations, while successfully
accounting for the instability against long-range positional
order and for the initial thermal disordering of the lattice.
Our model can be regarded in a similar way. A more complete treatment would require abandoning
the constraint of having six defined nearest neighbors,
and using pair potentials for the $AA$, $BB$, and $AB$ in-
teractions between the two kinds of atoms $A$ and $B$ in the
random alloy $A_{1-x} B_x$. The repulsive part of the pair poten-
tial will completely inhibit the pleating, but the possi-
bility of switching nearest neighbors leads to the flexibil-
ity of lowering the energy by creating disclinations, dislo-
cations, etc. Taking the thermal analogy seriously, such
excitations would be expected to be present in the ground
state as $T_D$ is increased.

Thermal effects can be incorporated into our model at
low temperatures. If the thermal and static displacements
are controlled by the same force constant $K$, then the
thermal and configurational averages can be done separ-
ately to give

$$ \eta = \frac{4q^2 k_B (T+T_D)}{3v^3} \pi K. $$

(36)

In the limit that $T_D$ goes to zero, the usual thermal result
is recovered.

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