Evaluation of phason elastic constants from HRTEM image of a dislocation in icosahedral quasicrystal

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Abstract. A method is proposed for quantitative evaluation of the ratio of the two phason elastic constants $K_2/K_1$ in icosahedral quasicrystals from a high-resolution transmission electron microscopy (HRTEM) image of a dislocation. Here, the Hytch’s method originally proposed for quantitative evaluation of displacement fields in crystals is generalized to quasicrystals. The generalized Hytch’s method gives phason displacement fields around a dislocation in quasicrystals, from which $K_2/K_1$ can be evaluated. This method is demonstrated using a simulated HRTEM image of a dislocation in an icosahedral quasicrystal.

Introduction

Quasicrystals have incommensurate structures in which the incommensurate length scales are determined by the geometrical constraints associated with non-crystallographic point group symmetry [1]. Originating in the incommensurability, quasicrystals have a special type of elastic degrees of freedom [2]. Quasicrystals are accompanied by the phason elastic constants. The generalized elasticity of quasicrystals is described in terms of the two types of elastic fields. Within a linear elasticity, icosahedral quasicrystals have five independent elastic constants: two ($K_1$ and $K_2$), to pure phason elasticities; and one ($K_3$), to a coupling between the two [3, 4].

The phason elasticity is closely related to the problem of what is the physical origin of the quasicrystalline structural order [5], and it has attracted much attention since the discovery of the quasicrystal. So far, experimental evaluations of the phason elastic constants have been done exclusively by diffuse scattering measurements of neutron or X-ray; the measurements have been reported for icosahedral quasicrystals of Al–Pd–Mn [6, 7], Al–Cu–Fe [8] and Zn–Mg–Sc [9] systems. In this paper, we propose and formulate another method for the evaluation of the phason elastic constants (more precisely their ratio $K_2/K_1$), in which we use a high-resolution transmission electron microscopy (HRTEM) image of a dislocation. Here, the method developed by Hytch et al. [10, 11] for quantitative evaluation of displacement fields in crystals is generalized and applied to the evaluation of the phason displacement field around a dislocation in quasicrystals. By comparing the evaluated phason field with the field derived theoretically, we can evaluate $K_2/K_1$.

Hytch’s method and its application to displacement fields around a dislocation in an icosahedral quasicrystal

Hytch et al. [10, 11] have developed a method for measuring displacement fields in crystals with high precision from HRTEM images. They have applied the method to the displacement fields around an edge dislocation in silicon and showed that the measured displacements agree with those expected by the anisotropic elastic theory to an accuracy of 0.003 nm. In this section, we briefly review the method and generalize it for the application to displacement fields around a dislocation in an icosahedral quasicrystal.

The intensity in a HRTEM image, $I(r)$, of a perfect crystal can be written as:

$$I(r) = \sum_g A_g \exp \left(2\pi i g \cdot r + iP_g(r)\right),$$

(1)

where $g$ are the reciprocal lattice vectors and $A_g = A_g \exp (iP_g)$ are the corresponding Fourier components. $I(r)$ of a distorted crystal can be described by assuming spatially varying Fourier components, i.e.,

$$I(r) = \sum_g A_g(r) \exp \left(2\pi i g \cdot r + iP_g(r)\right),$$

(2)

where $P_g(r)$ is related simply to the displacement field $u(r)$ as

$$P_g(r) = -2\pi g \cdot u(r).$$

(3)

In principle, we can extract $P_g(r)$ by image processings from $I(r)$ for any $g$. Equation (3) indicates that the two dimensional $u(r)$ can fully be determined from $P_{g1}(r)$ and $P_{g2}(r)$ for any set of non-parallel $g1$ and $g2$. 

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The image intensity $I(r)$ of a distorted quasicrystal can be described as:

$$I(r) = \sum_{\mathbf{G}} A_{\mathbf{G}}(r) \exp \left(2\pi i \mathbf{g} \cdot \mathbf{r} + iP_{\mathbf{G}}(r)\right),$$

(4)

where $P_{\mathbf{G}}(r)$ is given as:

$$P_{\mathbf{G}}(r) = -2\pi G \cdot U(r) = -2\pi (g_\parallel \cdot u(r) + g_\perp \cdot w(r)).$$

(5)

Here, $U = u + w$ is a high dimensional displacement vector, whose physical-space ($E_\parallel$) and complementary-space ($E_\perp$) components are $u$ and $w$, respectively; they correspond to the phonon and phason displacements. $G = g_\parallel + g_\perp$ represents a high dimensional reciprocal lattice vector, where $g_\parallel$ and $g_\perp$ are its physical-space and complementary-space components, respectively. The same image processings used for extracting $P_{\mathbf{G}}(r)$ in Eq. (2) for a crystal can be applied to extract $P_{\mathbf{G}}(r)$ in Eq. (4) for a quasicrystal, as demonstrated in the following section.

Yang et al. [12] have derived an analytical expression of displacement fields around a dislocation whose line direction is parallel to a fivefold axis in an icosahedral quasicrystal, on the assumption that the phonon-phason coupling is negligible\(^1\). Here, we consider such a dislocation. We further assume that the Burgers vector is $\mathbf{B} = (b_0, 00b_0, 00)$ (e-basis), where the first three indices represent the $E_\parallel$ components while the last three represent the $E_\perp$ ones\(^2\). The dislocation line direction in $E_\parallel$ is $\mathbf{l} = (001000)$ (e-basis) and therefore the dislocation considered here is of pure-edge type. Using the analytical expression derived by Yang et al. [12], we obtain the displacement field:

$$U = u_1u_2001w_200,$$

$$u_1 = \frac{b_0}{2\pi} \left[\theta + \frac{1}{4(1-v)} \sin (2\theta)\right],$$

$$u_2 = \frac{b_0}{2\pi} \left[\frac{1 - 2v}{2(1-v)} \ln \left(\frac{r}{r_0}\right) + \frac{1}{4(1-v)} \cos (2\theta)\right],$$

$$w_1 = \frac{b_0}{2\pi} \left[\theta + K \sin (4\theta)\right],$$

$$w_2 = \frac{b_0}{2\pi} K \left[4 \ln \left(\frac{r}{r_0}\right) + \cos (4\theta)\right],$$

$$K = \frac{g_2^2}{24 + 24 \left(\frac{K_2}{K_1}\right)^2 - 88 \left(\frac{K_2}{K_1}\right)^2}.$$

(6)

where $r$ and $\theta$ are the polar coordinates centered on the dislocation core, $r_0$ is the cut-off radius, $v$ is the Poisson's ratio, and $K_1$ and $K_2$ are the phason elastic constants. Here, we follow the definition by Widom [15] for $K_1$ and $K_2$, although Yang et al. [12] adopts the definition by Ding et al. [16]. This is because most of the papers reporting the evaluation of $K_1$ and $K_2$ by diffuse scattering measurements (e.g., [6–9]) follow the definition by Widom [15]. We note that the phonon displacement part in Eq. (5) is identical to the solution by the isotropic elastic theory for an edge dislocation.

In general, we can obtain $P_{\mathbf{G}}(r)$ in Eq. (5) by image processings for arbitrary $G$ having the form $G = (g_\parallel, g_\parallel, g_\perp, 0)$ (e-basis). In particular, for $G = (g_\parallel, 00, 00)$ (e-basis), Eq. (5) becomes:

$$P_{\mathbf{G}}(r) = - (g_\parallel b_\parallel + g_\perp b_\perp) \theta - \frac{g_\parallel b_\parallel^2}{4(1-v)} \sin (2\theta)$$

$$- g_\perp b_\perp K \sin (4\theta).$$

(7)

In addition, if we select $G$ so as to satisfy $g_\parallel b_\parallel + g_\perp b_\perp = 0$ (weak invisibility condition [17]), Eq. (7) reduces to:

$$P_{\mathbf{G}}(r) = - \frac{g_\parallel b_\parallel^2}{4(1-v)} \sin (2\theta) - g_\perp b_\perp K \sin (4\theta).$$

(8)

This $P_{\mathbf{G}}(r)$ consists only of two sinusoidal terms with different $\theta$ dependency, where the magnitude of the first term gives $\nu$ and that of the second term gives $K_2/K_1$. This indicates that we can evaluate those values from $P_{\mathbf{G}}(r)$.

**Demonstration of the method using a simulated HRTEM image**

In this section, we demonstrate the method described in the preceding section using a simulated HRTEM image. Figure 1 shows the simulated HRTEM image of an icosahedral quasicrystal, where a dislocation is introduced at the center of the figure. The dislocation line is along a fivefold axis of the icosahedral quasicrystal, which is parallel to the incident beam direction. In general, an HRTEM image corresponds to the projected structure along the incident beam direction, which should be a two

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\(^1\) It should be kept in mind that the coupling is not always negligible, as shown in [13, 14]. In principle, we can derive the equations corresponding to Eqs. (6)–(8) in this paper with non-zero coupling constant $K_3$, although they should have much more complicated forms.

\(^2\) In [12], two different types of coordinate system are used. One of them corresponds to the coordinate system used here, which we call 'e-basis' hereafter. The other is based on the six dimensional lattice translational vectors, which we will call 'd-basis'. $P_{\mathbf{G}}$ in Eq. (19) in [12] are the projections of them onto $E_\parallel$. 

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Fig. 1. The simulated HRTEM image of an icosahedral quasicrystal, where a dislocation is introduced at the center. This has been constructed using a rhombic Penrose tiling with the edge length of $a_0$. The size of the image is $46a_0 \times 46a_0$. 

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dimensional decagonal quasicrystalline structure in this case. We simulated the HRTEM image using a rhombic Penrose tiling known as a typical decagonal quasicrystal; we simply arranged Gaussian functions with a fixed width at the vertex points of the Penrose tiling to construct the image. The Burgers vector of the dislocation is \( \mathbf{B} = (001221) \) (\( d \)-basis) = \( \mathbf{a}_0 (0.45, 0, 0, -5.0, 0, 0) \) (\( e \)-basis), where \( \mathbf{a}_0 \) denotes the edge-length of the Penrose tiling. The \( E_\parallel \) component of \( \mathbf{B} \), i.e., \( b_\parallel \) is along the \( e_1 \) direction in Fig. 1. If you observe the figure at grazing angle, you will find distortions and jogs in lattice planes in the vicinity of the dislocation core. The ratio between \( E_\parallel \) and \( E_\perp \) components of \( \mathbf{B} \), i.e., \( |b_\parallel|/|b_\perp| \) equals to \( r^2 \) \( (r = (1 + \sqrt{5})/2) \). This type of Burgers vector has been observed frequently in icosahedral Al–Pd–Mn [18]. We assume \( v = 0.25 \) and \( K_2/K_1 = -0.52 \), which has been reported for the Al–Pd–Mn [7, 19].

We calculated the Fourier transform \( I(r) \) of the simulated HRTEM image after applying a von Hann function as a mask in real space to avoid streaking (Fig. 2). The reciprocal lattice vector satisfying the weak invisibility condition is \( \mathbf{G} = (002112) \) (\( d \)-basis), which is indicated by an arrow in Fig. 2. We applied a Gaussian mask to this spot and made the inverse Fourier transformation (Fig. 3). Here, there are no extra fringes inserted because of the weak invisibility condition. Finally, we subtracted \( 2\pi g_\parallel \cdot \mathbf{r} \) from the phase in the image of Fig. 3, the result of which is shown in Fig. 4. This map should represent \( P_0(r) \) in Eq. (8). We notice, however, that the map in Fig. 4 depends not only on \( \theta \) but also on \( r \) in a region close to the dislocation core. This could be attributed to the fact that in the core region magnitude of the strain is too large for this method to be applied. We have evaluated the \( \theta \) dependence in a region far apart from the dislocation core in the map of Fig. 4; the variation has been measured around the circle with radius of 13.5\( a_0 \) shown in Fig. 4, averaged over 1.35\( a_0 \) radially. The result is shown in Fig. 5 (solid line), which should be compared with the curve calculated by Eq. (8) with \( v = 0.25 \) and \( K_2/K_1 = -0.52 \) (broken line). The agreement between the two lines is quite satisfactory. Here, in addition to the main contribution by the phonon displacement part with sin \( (2\theta) \) dependence, the effect of the phason displacement part with sin \( (4\theta) \) dependence is clearly noticed; the sin \( (2\theta) \) variation leans slightly towards the small angles, i.e., the positive slope is steeper than the negative. This is due to the contribution of the sin \( (4\theta) \) term.

Conclusions

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quasicrystals from a high-resolution transmission electron microscopy image of a dislocation. Here, the Hytch’s method [10, 11] originally proposed for quantitative evaluation of displacement fields in crystals is generalized for the application to displacement fields around a dislocation in an icosahedral quasicrystal. The generalized Hytch’s method gives phason displacement field around the dislocation. By comparing the evaluated phason field with the field derived theoretically, we can evaluate $K_2/K_1$. We have demonstrated the method using a simulated image of a dislocation in an icosahedral quasicrystal and shown the validity of the method.

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