THE COMPARISON OF LATTICE AND CONTINUUM THEORIES
OF HUANG SCATTERING

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ABSTRACT

The predicted X-ray and neutron scattering by random semiconductor alloys $A_{1-x}B_xC$ with the zincblende structure, has been analyzed using direct simulation of the scattering from the atoms in the lattice, and also using continuum theory. This initial work has focused on the special case of the single impurity limit (small concentration x) where the elastic properties of both the pure crystals ($x = 0$ and $x = 1$) are isotropic and the same. The influence of different atomic scattering amplitudes on the intensity has also been analyzed. Distortions occur in the crystal caused by the size-mismatch of the impurity atoms, which results in diffuse scattering of which the most important component is the Huang scattering around the Bragg peaks. The Huang scattering has the shape of a double-drop and we obtain surprisingly good agreement between the continuum and lattice approaches. This is because long-wavelength concentration-waves make the dominant contribution to the divergent Huang scattering, with the remainder of the diffuse scattering being very weak.

I. INTRODUCTION

The theory of diffuse scattering from random alloys was developed many years ago. After the very important early work of Huang [1], a rather complete theory of the diffuse scattering from alloys was developed by Krivoglaz and coworkers [2-4] in the Ukraine. This pioneering work contains most of the formalism necessary to understand diffuse scattering in the continuum limit. An English translation of this work is now available in book form and is highly recommended to the interested reader [3]. Of particular interest to us in this paper is
the diffuse scattering in a semiconductor caused by a single impurity due to the lattice strain and the associated size-mismatch between the impurity and the host.

Modern simulation techniques on lattices allow the individual atomic displacements to be found and hence the associated diffuse X-ray or neutron scattering to be calculated. A crystalline alloy has a mean long range order that leads to Bragg peaks and the associated Huang scattering [1] is divergent very close to these Bragg peaks. In this paper we compare the lattice and continuum approaches and find that the continuum approach is remarkably good. This was anticipated near the Bragg peaks, but in fact the continuum is found to be a remarkably good approximation everywhere in the case of small defect concentration. This is because the lattice structure is only important at short wavelengths where the diffuse scattering is very weak anyway. Nevertheless the excellence of the continuum approximation was somewhat of a surprise to us.

In this paper, we first describe the lattice simulations in the next section. We look only at the special case of semiconductors with a single defect, where the elastic constants of the host and the defect are isotropic and the same. This is accomplished by using a Kirkwood model [5]. In section 3, we review the continuum approximation with a calculation for a single defect. In section 4, we compare results for the displacement field around the single defect, and in section 5, we compare the results for the diffuse scattering, using a variety of graphical representations. We end with a brief discussion.

Throughout this paper we consider only a single defect in a zincblende structure. This is the limit at a small concentration $x$ of the alloy $A_{1-x}B_xC$. We use masses that correspond to the alloy $Ga_{1-x}In_xAs$, and force constants in a Kirkwood model, which contains bond-stretching and angle-bending terms, where the force constants are chosen to give the elastic constants of GaAs, which we make isotropic for simplicity. This is an initial study, where we have simplified everything, except for the size-mismatch between the Ga and In ions which is the crucial ingredient.

2. LATTICE SIMULATIONS

The zincblende structure contains two sublattices, each with a face centered cubic structure. A single impurity is placed in one of these sublattices and the subsequent lattice relaxation and associated diffuse scattering is studied. The direct simulation of the scattering from the atoms in the lattice was based on a numerical procedure [6] which adjusts the positions of all atoms and the size of the cubic supercell to minimize the energy for an alloy $A_{1-x}B_xC$. The size-mismatch was described with a Kirkwood potential [5] following the
scheme of Thorpe and co-workers [6-9] for an A\textsubscript{1},B,C semiconductor alloy. The lattice contains two kinds of bonds between atoms from the two sublattices; the second sublattice being always occupied by C atoms. The distorted equilibrium structure is obtained by minimizing the energy associated with the Kirkwood potential [5]

$$V = \frac{\alpha}{2} \sum_{ij} \left( L_{ij} - L_{ij}^0 \right)^2 + \frac{\beta}{8} L_c^2 \sum_{i\neq jk} \left( \cos \theta_{ijk} + \frac{1}{3} \right)^2.$$  

(1)

Here $L_{ij}$ is the length of the bond $ij$ and $L_{ij}^0$ is the natural (unstrained) bond length $L_{ij}^0$, which can take on the values $L_{AC}^0$, $L_{BC}^0$ with probability $1 - x$ and $x$ respectively. The change of this bond length is related to the stretching force constant $\alpha$. The angle $\theta_{ijk}$ is the variable associated with the tetrahedral angle which has a natural (i.e. unstrained) value of $\cos^{-1}(-1/3) = 109^\circ$. The indices $j$, $k$ are nearest neighbors to the central atom $i$ as shown in Fig. 1(a). The change of the angle $\theta_{ijk}$ is controlled by the bending force constant $\beta$.

![Diagram](image)

**Fig. 1.** (a) A sketch of the tetrahedron surrounding the impurity atom in the zincblende structure and (b) the radial displacement field around the atom as obtained by the continuum theory.

In the first order approximation consistent with using a harmonic potential (1) the bond length can be written as

$$L_{ij} = L_c + \vec{r}_j \cdot \vec{u}_i,$$

(2)
where \( L_e \) is the nearest-neighbor distance of the undistorted virtual crystal, \( u_i \) is the displacement of site \( i \) from its position in the undistorted structure, and \( \tilde{u}_y = \tilde{u}_j - \tilde{u}_i \). The unit vector \( \hat{r}_{ij} \) joins sites \( i, j \) in the undistorted structure. We will take all the spring constants to be equal in this paper as it simplifies the analytical treatment, [9] and choose the ratio \( \alpha / \beta \) to correspond to isotropic elastic constants (which does not qualitatively influence the results). The isotropy condition \( c_{11} - c_{12} = 2c_{44} \) for the elastic constants is imposed so that we have the following relations between the elastic moduli and the force constants [9]

\[
c_{11} = \frac{1}{3a} \left( \alpha + 3\beta - \frac{\lambda}{3} \beta \right) \quad \text{and} \quad c_{12} = \frac{1}{3a} \left( \alpha - \beta - \frac{\lambda}{3} \beta \right),
\]

where \( \lambda = 1 \) and \( \alpha = 16\beta/9 \) for the Kirkwood model [5] (with \( \lambda = 0 \) for the Keating model [10], which we do not use here). For isotropic elastic moduli in crystalline Ga\(_{1-x}\)In\(_x\)As, we used the following values of the force constants: \( \alpha = 49.138 \) N/m; \( \beta = 27.64 \) N/m, leading to the elastic moduli \( c_{11} = 7.2432 \) dyn/cm\(^2\) with \( c_{12} = 0.1 \) \( c_{11} \), and hence a Poisson ratio \( \nu = 2c_{12} / c_{11} = 0.2 \). The unstrained length of the GaAs bond is \( a_2 = 2.4479\AA \) and the InAs bond is \( a_1 = 2.6233\AA \), so we use atomic radii of 1.2124\AA\, 1.3878\AA\ and 1.2355\AA\ for the Ga, In and As ions respectively. The mismatch in length of the InAs bond compared with the GaAs bond is about 7%.

The scattering intensity was computed from the relaxed coordinates using the expression [11]

\[
I(\vec{Q}) = \left| \sum_i f_i \exp(i\vec{Q} \cdot \vec{R}_i) \right|^2
\]

where \( I(\vec{Q}) \) is the total scattering intensity, and \( \vec{Q} \) is the diffraction vector, \( \vec{Q} = \vec{k}_i - \vec{k}_o \), and \( \vec{k}_i \, \vec{k}_o \) are the wavevectors of scattered, incident wavevectors respectively with \( |\vec{k}_i| = |\vec{k}_o| = 2\pi / \lambda \), where \( \lambda \) is the X-ray, or neutron, wavelength. We also will use the quantity \( \vec{q} = \vec{Q} - \vec{G} \), to describe the scattering around a single reciprocal lattice vector \( \vec{G} \). The factor \( f_i \) is the strength of the scattering from an individual atom \( i \), and is the atomic form factor for X-ray scattering (which goes like the atomic charge \( Z \) at small wavevector \( Q \)) and the neutron scattering length for neutron scattering.
For a direct computer simulation of the scattering intensity by random semiconductor alloys with the zincblende structure, we used a supercell with $L \times L \times L$ cubes of the zincblende structure, each containing 8 atoms, and with periodic boundary conditions. A single impurity atom was placed in this large supercell. Different supercell sizes were used for direct simulations over the lattice to evaluate the influence of the size of the supercell on the accuracy of the calculation of the displacement field and diffuse scattering intensity, and in order to obtain a denser mesh of points for the calculation of the diffuse scattering. The simulation program, which used a variant of the conjugate gradient method, [6] adjusted the positions of all atoms and the size of the supercell to minimize the energy. The simulation was terminated when the strain energy had converged to better than 1%. It was found that $L = 40$, which corresponds to 512,000 atoms in the supercell, was plenty large enough and is used throughout this paper. The supercell was kept strictly cubic and its size scaled by the mean bond length as required by Vegard’s law, which is known to hold strictly for the conditions here (no force constant disorder [9]). The mean bond length [9] is given by Vegard’s law [12]

$$\langle L \rangle = (1-x)L_{AC}^0 + xL_{BC}^0.$$  \hspace{1cm} (5)

Although the defect concentration $x = 1/256,000$ is very small in this calculation, it is important to make this adjustment to the sample size, using (5), as the diffuse scattering is only meaningful at the superlattice points in reciprocal space associated with the supercell, and we found that it was important to be exactly at these points. Note that we use the full expression (4) for the scattered intensity with these lattice calculations and make no assumptions about small displacements and expanding the expression (4) as is done in the continuum theory.

3. CONTINUUM THEORY

The continuum theory of diffuse scattering from isolated defects [2-5, 13-16] gives a detailed analysis of isodiffuse surfaces types in the vicinity of reciprocal lattice sites for cubic crystals. This theory has been worked out for a wide variety of geometries and defect types and is summarized in a recent book [3]. We will present here a simple derivation of the isotropic case of interest to us in this paper.

Consider an elastic sphere with radius $R_1$, subject to an external hydrostatic pressure $P_1$. The displacement $\vec{u}_i$ is only in the radial direction inside the sphere, is linear in $r$, and can be easily calculated using continuum mechanics [17] as
\[ \bar{u}_1 = -\frac{P_1}{3K} \hat{r}, \]  

(6)

where \( K \) is the bulk modulus of the material. We now consider the \textit{inverse} situation, of an infinite elastic continuum, containing a spherical hole of size \( R_2 \), with an inside hydrostatic pressure \( P_2 \). In this case the displacement field \( \bar{u}_2 \) is also radial and is given by an inverse square behavior with distance

\[ \bar{u}_2 = \frac{P_2 R_1^3}{2\mu r^3} \hat{r}, \]  

(7)

where \( \hat{r} \) is a unit vector along \( \bar{r} \). We assume that \( R_1 > R_2 \), and put the larger sphere inside the smaller spherical hole. The boundary conditions are that the pressure is continuous and the radial displacement field is continuous. These two conditions lead to the pressure at the boundary

\[ P = P_1 = P_2 = \frac{R_1 - R_2}{R_2/4\mu + R_1/3K}. \]  

(8)

Of most interest to us here is how the displacement field falls off outside the impurity, and this is given by

\[ \bar{u}_2 = \frac{R_1 - R_2}{R_2/4\mu + R_1/3K} \frac{R_2^3}{2\mu r^3} \hat{r}. \]  

(9)

Note that the bulk modulus \( K \) is associated with the \textit{inner} material and the shear modulus \( \mu \) with the \textit{outer} material, although here we do not make any distinction in this paper as the two materials are assumed to be the same elastically. We can rewrite the result (9) in a more convenient form if we use the fact that the difference \( \Delta R = R_1 - R_2 \) is small, and also use the Poisson ratio \( \nu \) as given by \( K/\mu = \frac{3}{2}(1+\nu)/(1-2\nu) \) so that (9) becomes

\[ \bar{u}_2 = \frac{\Delta R}{3R} \left( \frac{1+\nu}{1-\nu} \right) \frac{R_2^3}{12\pi r^3} \hat{r} = \frac{\Delta V}{12\pi r^3} \left( \frac{1+\nu}{1-\nu} \right) \hat{r}. \]  

(10)
which depends only on two parameters; \( \Delta V \) the change in volume associated with the mismatch, and the Poisson ratio \( \nu \). A sketch of this displacement field around the impurity is shown in Fig. 1(b), which shows the \( 1/r^2 \) behavior outside the sphere.

The scattering amplitude can be found from the Fourier transform \( \tilde{\mathbf{u}}_q \) of the displacement field. We neglect the displacement field \( \tilde{\mathbf{u}}_i \) inside the sphere, and calculate \( \tilde{\mathbf{u}}_q \) as

\[
\tilde{\mathbf{u}}_q = \int \tilde{\mathbf{u}}_2 \exp(i\mathbf{q} \cdot \mathbf{r}) d^3r / V_a = i \frac{\Delta V}{V_a} \frac{\mathbf{q} \cdot \mathbf{q}}{q^3(1-\nu)}
\]

where \( V_a \) is the volume per atom (i.e. the volume of the sample divided by the total number of atoms including both sublattices). The expression above is only meaningful for small wavevectors \( q \) as we are in the continuum limit.

The expression for the scattered intensity (4) can be rewritten using the equilibrium positions in the virtual crystal \( \bar{\mathbf{R}}_i^o \), where \( \bar{\mathbf{R}}_i = \bar{\mathbf{R}}_i^o + \mathbf{u}_i \), as

\[
I(\bar{\mathbf{Q}}) = \left| \sum_i \exp(i\mathbf{Q} \cdot \bar{\mathbf{R}}_i^o) \exp(i\mathbf{Q} \cdot \mathbf{u}_i) \right|^2 \\
= \left| \sum_i \exp(i\mathbf{Q} \cdot \bar{\mathbf{R}}_i^o) [1 + i\mathbf{Q} \cdot \mathbf{u}_i] \right|^2 \\
= \left| \sum_i \exp(i\mathbf{Q} \cdot \bar{\mathbf{R}}_i^o) \right|^2 + \left| \mathbf{Q} \cdot \mathbf{u}_q \right|^2 \\
= I_b(\mathbf{Q}) + I_h(\mathbf{Q})
\]

where we have set all the amplitude factors \( f_i \) in (4) equal to unity for the present. The first term in (12) is the Bragg scattering \( I_b(\mathbf{Q}) \) associated with the virtual crystal and the second term is the Huang scattering \( I_h(\mathbf{Q}) \), where we have taken only the leading non-zero term in (12) which is dominant. Note that the wavevector \( \bar{\mathbf{Q}} \) is associated with each reciprocal lattice vector in turn via \( \bar{\mathbf{q}} = \mathbf{Q} - \mathbf{Q} \). Using Eqns. (11) and (12), the Huang scattering in the continuum limit is
\[ I_n(\vec{Q}) = \left[ \left( \frac{\Delta V}{V_a} \right) \left( \frac{1 + \nu}{3(1 - \nu)} \right) \left( \frac{\vec{Q} \cdot \vec{q}}{q} \right) \right]^2 \]  

for a single defect. In the low concentration limit, the scattering from isolated defects will be additive, and so the above expression would just be multiplied by the number of defect atoms to get the total scattering. Note that the first factor in (13) is just the relative size change associated with the impurity atom where \( \Delta V / V_a = 3 \Delta R / R \). Note also that this is the change in the natural length associated with the substitution of a host atom with an impurity and not the actual length change, which in general will be smaller in magnitude, because of the restraining effect of the rest of the lattice.

For a small concentration of defects in an elastically isotropic medium in the vicinity of reciprocal lattice sites, classic Huang scattering occurs as found by many previous authors [2-4, 13-16] whose result we reproduce here

\[ I_n(\vec{Q}) = N_d |f|^2 e^{-2W} \left( \frac{1}{V_i} \frac{dV_i}{dx} \right)^2 \left( \frac{1 + \nu}{3(1 - \nu)} \right) \left( \frac{Q^2 \cos^2 \theta}{q^2} \right), \]  

which is proportional to \( \cos^2 \theta \), where \( \theta \) is the angle between \( \vec{Q} \) and \( \vec{q} \). This results in the appearance of similar strong Huang scattering around all reciprocal lattice points having the shape of a double-drop. In the expression (14), \( N_d \) is the number of defects and \( f \) is an average scattering factor that has been put back. The Debye-Waller factor involving \( W \) can be ignored for a single defect as it is a \( 1/N \) effect, where \( N \) is the total number of atoms. The quantity \( V_i \) is the total volume of the crystal and so using Vegard’s law (5), we see that Eqn. (14) indeed reduces to (13) in the appropriate limit as expected, including the overall normalization. We have found the simple calculation of Huang scattering given in this section instructive, and perhaps simpler than some of the traditional calculations that have led to (14).

In the case when all the scattering factors \( f_i \) in (4) are not all set equal to unity, the separation into Bragg and Huang scattering in (12) must be done with more care [2-4]. In particular there are the main Bragg peaks that we have been discussing, with their associated diffuse scattering \( I_D(\vec{Q}) \) given by

\[ I_D(\vec{Q}) = \left[ \frac{1}{2} \left( \frac{\Delta V}{V_a} \right) \left( \frac{1 + \nu}{3(1 - \nu)} \right) \left( \frac{\vec{Q} \cdot \vec{q}}{q} \right) + (f_A - f_S) \right]^2, \]  

(15)
where the diffuse scattering \( I_D(\vec{Q}) \) becomes the Huang scattering \( I_H(\vec{Q}) \) as given in (12) and (13) when all the atomic scattering factors \( f_i \) are set equal to unity. In general the diffuse scattering in (15) contains the divergent Huang amplitude and another non-divergent amplitude, which increases the scattering slightly on one side of the peak and decreases it on the other.

When \( f_A \neq f_C \) additional Bragg peaks occur. These are the extra peaks that are observed in the zincblende structure but not seen in the diamond structure. There is diffuse scattering associated with these peaks also, which has the form

\[
I_D(\vec{Q}) = \left( \frac{(f_A - f_C)}{2} \left( \frac{\Delta V}{V_a} \right) \left( \frac{1 + v}{3(1 - v)} \right) \left( \frac{\vec{Q} \cdot \vec{q}}{q} \right) + (f_A - f_S) \right)^2,
\]  

and disappears completely when all the scattering factors are set equal to unity. Note that the diffuse scattering in (15) is associated with Bragg peaks whose intensity scales as \( (f_A + f_C)^2 \), whereas the diffuse scattering in (16) is associated with the weaker Bragg peaks whose intensity scales as \( (f_A - f_C)^2 \). Note that the Huang part of the diffuse scattering scales quadratically with the atomic form factor in the same way as the Bragg peak with which it is associated. So if one is strong so is the other and vice versa.

4. DISPLACEMENT FIELD

For defects in an elastically isotropic medium, the substitution of the host atom by an impurity atom is accompanied by the action of hydrostatic pressure on the surface of the impurity atom due to the size mismatch of host and impurity atoms, in the continuum viewpoint. This results in the appearance of an inverse square type displacement field in the matrix as sketched in Fig. 1(b) decreasing as \( 1/r^2 \) with the distance \( r \) between the defect and the matrix site, as discussed in the previous section.

There is a question as to the proper choice of the length change \( \Delta R \) or equivalently the volume change \( \Delta V \) associated with the defect that should be used in Eqn. (10). This forms the bridge between the continuum theory and the lattice simulations. The volume associated with the GaAs bond length \( a_2 \) is \( 4\pi a_2^3 / 3 \) so that \( \Delta V = 4\pi (a_1^3 - a_2^3) / 3 = 14.2 \text{ Å}^3 \). This is clearly too large when compared with Figs. 2(a) and (3).
Fig. 2. Showing (a) the radial $U = \vec{u} \cdot \vec{r}$ and (b) the tangential $T = |\vec{u} \times \vec{r}|$ parts of the displacement field calculated by direct simulation over the lattice (solid dots) and calculated from the continuum theory given in Eqn. (10) for a single defect using the continuum approach. Note that the tangential displacements are ten times smaller and predicted to be zero by the continuum theory. The distance $r$ is measured in Angstroms.

The proper procedure [2, 3] is to take the Wigner-Seitz cell surrounding the Ga ion, and ignoring the As ions, to give a volume of $16a_2^3/3\sqrt{3}$, and hence $\Delta V = 16(a^3_1 - a^3_2)/3\sqrt{3} = 10.4 \, \text{Å}^3$ which gives a better fit to the lattice simulation data. Actually the best fit is given by the linearized version of this result $\Delta V = 16a_2^3(a_1 - a_2)/\sqrt{3} = 9.71 \, \text{Å}^3$ which is what we use in Eqn. (10) and is shown as the lines in Figs. 2(a) and 3.

Fig. 3. Showing an enlargement from Fig. 2(a) of the radial $U = \vec{u} \cdot \vec{r}$ part of the displacement field calculated by direct simulation over the lattice (solid dots) and calculated from the continuum theory given in Eqn. (10) for a single defect using the continuum approach. The distance $r$ is measured in Angstroms.

To check the type of displacement field caused by In atoms in a GaAs matrix with the ratio between bond stretching and bond bending force constants $\alpha / \beta$ corresponding to an isotropic elastic medium, we have simulated the displacement field for such a crystal with one In atom substituted for a GaAs atom and with a size of $40 \times 40 \times 40$ cells with 512,000
atoms. The change of the radial and tangential parts of displacement field with the distance from the impurity atoms are shown in Figs. 2(a) and 2(b). We have verified that the displacement field falls off as an inverse square law at large distances from the single defect as predicted by continuum theory, but that there are significant deviations close to the defect. The theoretical curve corresponding to Eqn. (6), with no adjustable parameters, is shown by a solid line, the results of simulation are presented by dots. In Fig. 3, we show an enlargement of Fig. 2(a) which shows that there are small but real fluctuations away from the inverse square behavior at all distances.

It is seen that tangential part of the displacement field is ten times smaller than radial component, so that we can use this approximation and consider that displacement field created by In impurity atoms as being of an inverse square type. The deviation of the displacement field from a pure inverse square in the several nearest neighbors will influence the intensity distribution at large distances from the reciprocal lattice points, while in the vicinity of a reciprocal lattice point, the scattered intensity is caused mainly by the atoms relatively distant from the defect (where the inverse square type of displacement field is good, on average).

![Contour maps of the diffuse scattering, from lattice simulations, for a single In defect in GaAs with isotropic elastic properties. In (a) the contours are for equal scattering amplitudes $f_A = f_B = f_C = 1$ and (b) with different scattering amplitudes $f_A = 31, f_B = 49$ and $f_C = 33$. The intensity is normalized by $(f_A + f_C)^2/4$.](image)
The deviations from the inverse square law shown in Fig. 2(a) and 3 are real and not due to any numerical noise or error, as we have checked this with different supercell sizes, and obtained identical results. These deviations appear to cancel out in the Huang scattering almost completely as seen in the next section. Such deviations may be enhanced by the two sublattice nature of the zincblende structure, where internal displacements inside the unit cell are allowed.

5. DIFFUSE SCATTERING

In this section, we give results for the diffuse scattering associated with a single In defect in a GaAs host, with all the force constants $\alpha$ and $\beta$, the same and chosen to give isotropic elastic behavior as described previously. All the lattice simulations are over a 512,000 atom supercell and the continuum calculations are described in section 3.

Again we must select the appropriate value of the relative volume change $\Delta V/V_0$, for use in Eqn. (13). From the previous discussion, this is associated with the change in the natural bond lengths of InAs and GaAs and hence $\Delta V/V_0 = (a_i/a_s)^3 - 1 = 0.231$. As before we find that the linear result, $\Delta V/V_0 = 3[(a_i/a_s)^3 - 1] = 0.215$ gives a slightly better fit when used in Eqn. (13) to fit the lattice simulations of the diffuse scattering as shown in Figs. 4, 6 and 7.

\[\text{Fig. 5. Showing the spatial distribution of the total scattered intensity, } I, \text{ from the lattice simulations, for a single In defect in GaAs with isotropic elastic constants with (a) equal scattering amplitudes } f_a = f_b = f_c = 1 \text{ and (b) with different scattering amplitudes } f_a = 31, f_b = 49 \text{ and } f_c = 33. \text{ The intensity is normalized by } (f_a + f_b)^2/4.\]

To get an overview of the scattering, we show in Fig. 4 a contour map of lines of equal intensity for the diffuse scattering. These were calculated from the lattice simulation, using the relaxed atomic coordinates and Eqn. (4). These contours are calculated for the (001) plane for the case when the change in scattering amplitude is neglected ($\Delta f = 0$) (a) and for
different scattering amplitudes with $\Delta f \neq 0$ (b). The double drop shapes around the (200), (020), (110) and (220) reciprocal lattice points, are aligned so that the axes point towards the origin. Slight anisotropy of the contours is caused by $\tilde{Q}$ being larger on the distant side of the reflection. It can be seen from Fig 4(b) that the difference of scattering amplitudes switches the anisotropy of the intensity distributions in the vicinity of reciprocal lattice points, while at large distances the scattering is almost same. Notice that the smaller Bragg peaks that scale as $(f_a - f_c)^2$ together with their associated Huang scattering, are just visible in Fig. 4(b). The wavevector $\tilde{Q}$ is in units of $4\pi/a_z$ in Figs. 4 - 8.

In Fig. 5 we show a different representation of the same results as in Fig. 4, but also include the Bragg peaks this time. It can be seen that additional smaller Bragg peaks occur when the scattering amplitudes are not the same as this corresponds to the difference between the zincblende and diamond structures. In particular, we see the appearance of additional Bragg peaks in the positions corresponding to the reflections (100), (010), (210), (120). Notice that the Huang scattering around the large peaks in Fig. 5(b) is substantial as predicted by (15) and extremely weak around the smaller Bragg peaks as predicted by (16).

Fig. 6. Showing the profile of the Huang scattering intensity from a single In defect in GaAs with isotropic elastic constants, for the (200) reflection along the [100] direction for different values of $q_z$ which is perpendicular to the $x$ direction. The lines are from the continuum theory and the corresponding symbols are from the lattice simulation. The values of $q_z$ are (0) 0, (1) 0.0125G, (2) 0.025G and (3) 0.0375G, where $G = 4\pi/a_z$, and the nearest neighbor bond length is $\sqrt{3}a_z/4$. The left panel (a) shows the case for equal scattering $f_a = f_b = f_c = 1$, and the right panel (b) for different scattering amplitudes $f_a = 31, f_b = 49$ and $f_c = 33$. The intensity is normalized by $(f_a^2 + f_b^2 + f_c^2)/4$.

In Fig. 6, we show the results of the direct lattice simulations (solid symbols) and the continuum result (solid lines) for the (200) strong Bragg reflection for different sections along the direction [100], which show remarkably good agreement with each other, not only for the
section passing through the center of the reflection but also through the side parts of it. We observe the decrease of the intensity in the central part of these distributions for a side section typical for the double-drop shape of the reflection. The anisotropy of the profiles is different for the case (a) with \( \Delta f^2 = 0 \), and compared with Eqn. (15) and in the case (b) with \( \Delta f^2 \neq 0 \) and compared with Eqn. (16). The short wavelength concentration waves, that are very different in the lattice and continuum theories, are only important when the scattering is weak out in the wings of the Huang scattering, and so in fact are seen to be largely irrelevant. Nevertheless it was not clear to us before doing this study that the continuum approach would be so spectacularly good.

In Fig. 7, we show the Huang scattering increases as the scattering vector \( Q \) increases in a quadratic way as \( Q^2 \) for both the strong and weak series of Bragg peaks separately. The diffuse scattering associated with the strong Bragg peaks is compared to the continuum theory in Eqn. (15) and that associated with the weak Bragg peaks is compared to the continuum theory in Eqn. (16).

![Graph showing intensity profile along [100] direction for higher orders of reflection (200) for a single In defect in GaAs with isotropic elastic constants and equal scattering amplitudes \( f_a = 31, f_b = 49 \) and \( f_c = 50 \). We have made \( f_c \) larger to emphasize the diffuse scattering around the smaller peaks. The lines are from the continuum theory and the corresponding symbols are from the lattice simulation. The intensity is normalized by \( (f_a + f_c)^2/4 \). The lines alternate strong, weak etc.]

The agreement of the lattice simulations with the continuum approximation is very good in all cases. Finally in Fig. 8, we show a blow up of the diffuse scattering associated with one of the weak Bragg peaks in Fig. 7, which shows some deviations with the
continuum theory. This is not unexpected as the scattering is very weak and continuum theory is after all only an approximation to the lattice.

The second non-divergent terms in Eqns. (15) and (16) do have small but observable effects on the intensity in the wings of the Huang scattering as can be seen in Figs. 4 - 8. These terms can be thought of as providing a background scattering everywhere. However because they add as amplitudes and not intensities, they can cause an asymmetry in the wings of the Huang scattering as shown for example in Fig. 8.

![Graph showing intensity vs. Qx](image)

**Fig. 8.** *An expanded view of the diffuse scattering associated with one of the weak Bragg peaks in Fig. 7. The intensity is normalized by (f_A+f_C)^2/4.*

### 6. DISCUSSION

The presence of isolated defects in a semiconductor crystal results in the appearance of intensive Huang scattering around the reciprocal lattice points. The intensity distribution of Huang scattering for defects in these cubic crystals, with isotropic elastic constants behaves as \((\tilde{Q}.\tilde{q})^2 / q^4\), where \(\tilde{Q}\) is the scattering wavevector and \(\tilde{q} = \tilde{Q} - \tilde{G}\) is measured from the reciprocal lattice point \(\tilde{G}\) of interest. The diffuse scattering is dominated by the Huang component and results in the double-drop shape of the isodiffuse surfaces. Results of a continuum theory of Huang scattering in the very low concentration limit, coincide with those for a relaxed lattice model studied here. Huang scattering is expected to be dominated by long wavelengths near the peaks in the scattering, so that continuum theory should provide a good description of the scattered intensity. We show that the strong, weak Bragg peaks have strong, weak diffuse scattering associated with them.

It is a bit of a surprise that continuum theory also does rather well in the wings of the Huang scattering, where shorter wavelengths are important, but this is because the scattering
is very weak and featureless. The displacement field associated with a single defect does fall off as an inverse square law on average, but with some deviations about the average due to the lattice structure. This is the first of a series of studies that we are undertaking to evaluate the continuum approximation to diffuse X-ray and neutron scattering in semiconductor alloys. Future work will consider higher concentrations of defects, cubic rather than isotropic elastic symmetry, and the effects of differences in the force constants between the host and the impurities.

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