

## ATOMIC MODELS OF DISLOCATIONS FOR SI AND GAAS

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**Key words:** Atomic models, dislocations, face centered cubic crystals, diamond, zincblende.

**Abstract.** *An atomic model of dislocations in face centered cubic crystals with a two-atom basis is proposed. This model has the standard cubic anisotropic elasticity as its continuum limit, and its main ingredients are the elastic stiffness constants and a dimensionless periodic function that restores the translation invariance of the crystal and influences the dislocation size. Possible applications include semiconductor materials such as silicon and GaAs.*

## 1 INTRODUCTION

Silicon and gallium arsenide are semiconductors of great importance for industry that crystalize in the face centered cubic (fcc) system. Crystals of these materials can be described as a fcc Bravais lattice with a basis of two atoms per site, which constitute a diamond structure for Si and a Zincblende structure for GaAs [1]. When growing layers of these materials, defects are very important because they act as nucleation sites, and have to be eliminated after the growth process has ceased. Among defects, dislocations and misfit dislocations are often observed [2, 3, 4]. Thus, it is desirable to have an economic description of these defects and their dynamics in terms of control parameters such as temperature [5]. A molecular dynamics description is very costly if we need to couple atomic details in the nanoscale to a mesoscopic description in larger scales that are important in the growth process [6]. In this work, we propose atomic models of defects and their dynamics that are vastly simpler than molecular dynamics, yet incorporating crystallographic details that are important for semiconductor growth.

We follow previous work for sc, fcc and bcc cubic crystals with an atom per lattice site [7]. Having two or more atoms per site introduces new features that are better explained revisiting the classic Born-von Karman work on vibrations of a linear diatomic chain[8]. In Section 2, we show how to obtain the wave equation for acoustic phonons in the elastic limit, directly from the equations for the diatomic chain. A similar calculation allows us in Section 3 to obtain the Cauchy equations for anisotropic elasticity in the continuum limit of our atomic models, which are constructed with the aim of having exactly this property. Section 4 shows how to calculate static dislocations for GaAs and Si. The last Section contains our conclusions.

## 2 CONTINUUM LIMIT FOR THE LINEAR DIATOMIC CHAIN

We shall consider a diatomic chain comprising alternatively atoms of masses  $M_1$  and  $M_2$  whose equilibrium positions are separated a distance  $s/2$ . The atoms are restricted to move only along the length of the chain. Their displacement with respect to their equilibrium positions will be denoted by  $u_l$  and  $v_l$ , respectively, in which  $l$  is the cell index. If  $\phi$  is the quadratic potential of interaction between neighboring atoms, the equations of motion for the diatomic chain are [8]

$$M_1 \ddot{u}_l = \phi' \left( v_l - u_l + \frac{s}{2} \right) - \phi' \left( u_l - v_{l-1} + \frac{s}{2} \right) = \phi'' \left( \frac{s}{2} \right) [(v_l - u_l) - (u_l - v_{l-1})], \quad (1)$$

$$M_2 \ddot{v}_l = \phi' \left( u_{l+1} - v_l + \frac{s}{2} \right) - \phi' \left( v_l - u_l + \frac{s}{2} \right) = \phi'' \left( \frac{s}{2} \right) [(u_{l+1} - v_l) - (v_l - u_l)]. \quad (2)$$

If we assume that the solutions of these equations are plane waves,

$$u_l = U e^{i(2\pi\eta l - \omega t)}, \quad v_l = V e^{i(2\pi\eta l - \omega t)}, \quad (3)$$

the following dispersion relation is obtained

$$\omega^2 = \frac{\phi''(s/2)}{M_1 M_2} [(M_1 + M_2) \mp \sqrt{(M_1 + M_2)^2 - 4M_1 M_2 \sin^2 \pi \eta}], \quad (4)$$

in which the minus (resp., plus) sign corresponds to the acoustic (resp., optic) branch of the dispersion relation [8]. Moreover, the corresponding amplitude ratio for the acoustic branch is

$$\frac{U}{V} = \frac{-M_2 (1 + e^{-i2\pi\eta})}{(M_1 - M_2) - \sqrt{(M_1 + M_2)^2 - 4M_1 M_2 \sin^2 \pi \eta}}, \quad (5)$$

with a similar formula for the optical branch [8]. In the long wavelength limit,  $\eta \rightarrow 0$ , the acoustic vibrations satisfy

$$U = V, \quad \omega = c \frac{2\pi\eta}{s}, \quad (6)$$

$$c = \sqrt{\frac{\phi''(s/2) s^2}{2(M_1 + M_2)}} = \sqrt{\frac{E}{\rho}}, \quad (7)$$

$$\rho = \frac{M_1 + M_2}{s}, \quad E = \frac{\phi''(s/2) s}{2}. \quad (8)$$

In these equations,  $E$  and  $\rho$  are the Young modulus and the linear mass density, respectively [8]. In the limit as  $\eta \rightarrow 0$ , each cell comprising two atoms moves rigidly with a phase velocity  $c$  and a wave number  $2\pi\eta/s$ .

The continuum limit of the diatomic chain equations recovers the acoustic vibrations only. In this limit,  $l \rightarrow \infty$  and  $s \rightarrow 0$ , with fixed  $x = ls$ . Furthermore,

$$u_l(t) = u(ls, t) = u(x, t), \quad v_l(t) = u\left(ls + \frac{s}{2}, t\right) = u\left(x + \frac{s}{2}, t\right). \quad (9)$$

If we now add Eqs. (1) and (2) divide by  $s$ , and use (9) to approximate the result, we obtain the following wave equation in the continuum limit:

$$\rho \frac{\partial^2 u}{\partial t^2} = E \frac{\partial^2 u}{\partial x^2}, \quad (10)$$

provided  $\rho$  and  $E$  are given by Eq. (8). The wave speed  $c$  is then given by Eq. (7). Equation (10) is the elastic continuum limit of the diatomic chain equations, *which does not contain optical vibrations*.

### 3 ATOMIC MODEL FOR A FCC LATTICE WITH A TWO-ATOM BASIS

In this Section, we propose an atomic model for a fcc lattice with a basis comprising two atoms, of masses  $M_1$  and  $M_2$ , respectively. Although this model is much more complicated to describe, the key ideas to show that it is compatible with anisotropic elasticity are the same as in Section 2 for the diatomic chain.

The main ideas needed to write a model for this crystal structure are the following:

1. Write the strain energy corresponding to a fcc crystal in a non-orthogonal basis with axes given by the usual primitive directions of the fcc Bravais lattice.
2. Write the corresponding strain energy for a fcc crystal with two atoms per lattice site.
3. Restore the periodicity of the crystal by defining the discrete distortion tensor as a periodic function (with period 1) of the discrete gradient of the displacement vector.
4. Define the potential energy of the crystal as the strain energy times the volume of the unit cell summed over all lattice sites. Then write down the equations of motion for the displacement vectors at each site.
5. Check that the continuum limit of the model yields the usual anisotropic elasticity.

We shall now carry out this program, which is an extension of that presented in Ref. [7] for a fcc lattice with a single atom per site. The primitive vectors of the fcc lattice are

$$a_1 = \frac{a}{2}(0, 1, 1), \quad a_2 = \frac{a}{2}(1, 0, 1), \quad a_3 = \frac{a}{2}(1, 1, 0), \quad (11)$$

in terms of the usual orthonormal vector basis  $e_1, e_2, e_3$  determined by the cube sides of length  $a$ . Let  $x_i$  denote coordinates in the basis  $e_i$ , and let  $x'_i$  denote coordinates in the basis  $a_i$ . Notice that the  $x_i$  have dimensions of length while the  $x'_i$  are dimensionless. The matrix  $T = (a_1, a_2, a_3)$  whose columns are the coordinates of the new basis vectors in terms of the old orthonormal basis can be used to change coordinates as follows:

$$x'_i = T_{ij}^{-1}x_j, \quad x_i = T_{ij}x'_j. \quad (12)$$

Throughout this paper, we use the Einstein convention of summing over repeated indices. Similarly, the displacement vectors in both basis are related by

$$u'_i = T_{ij}^{-1}u_j, \quad u_i = T_{ij}u'_j, \quad (13)$$

and their partial derivatives obey

$$\frac{\partial}{\partial x'_i} = T_{ji} \frac{\partial}{\partial x_j}, \quad \frac{\partial}{\partial x_i} = T_{ji}^{-1} \frac{\partial}{\partial x'_j}. \quad (14)$$

Again notice that  $u_i$  has dimensions of length, whereas  $u'_i$  is dimensionless. By using these equations, the strain energy density  $W = (1/2)c_{ijkl}e_{ik}e_{lm}$  can be written as

$$W = \frac{1}{2}c_{ijlm} \frac{\partial u_i}{\partial x_j} \frac{\partial u_l}{\partial x_m} = \frac{1}{2}c'_{rspq} \frac{\partial u'_r}{\partial x'_s} \frac{\partial u'_p}{\partial x'_q}, \quad (15)$$

where the new elastic constants are:

$$c'_{rspq} = c_{ijlm} T_{ir} T_{sj}^{-1} T_{lp} T_{qm}^{-1}. \quad (16)$$

To derive these equations, we have used the definition of the linear strain tensor  $e_{ik}$  as the symmetric part of the distortion tensor  $\partial u_i / \partial x_k$ , and the symmetry of the tensor of elastic constants,  $c_{ijklm}$ . Both  $c_{ijklm}$  and  $c'_{ijklm}$  have dimensions of force per unit area.

Once we have written the strain energy of a fcc crystal in the non-orthogonal basis spanned by the primitive vectors, we can introduce our discrete model. We shall consider a fcc lattice with a two-atom basis. In equilibrium, atoms with mass  $M_1$  will be placed at the lattice sites, so that their displacement vectors will depend on integer numbers and time:  $u'_i = u'_i(l, m, n; t)$ . In equilibrium, atoms with mass  $M_2$  will be placed at the sites of a fcc lattice which, in the orthonormal basis  $e_i$ , is rigidly displaced by a vector  $\Delta = (a/4, a/4, a/4)$  with respect to the first fcc lattice; see Fig. 1. In terms of the non-orthogonal basis  $a_i$ , the vector  $(a/4, a/4, a/4)$  becomes  $\Delta' = (1/4, 1/4, 1/4)$ . Thus the displacement vectors of the atoms with mass  $M_2$ ,  $v'_i = v'_i(l, m, n; t)$ , will be zero at equilibrium positions given by  $(l + 1/4, m + 1/4, n + 1/4)$  with respect to the lattice sites  $r' = (l, m, n)$  at which  $u'_i = 0$ . Apart from  $\Delta'$ , Fig. 1 shows that the following three vectors join the atom located at  $r'$  to three neighboring atoms with mass  $M_2$ :

$$b'_1 = \left(-\frac{3}{4}, \frac{1}{4}, \frac{1}{4}\right), \quad b'_2 = \left(\frac{1}{4}, -\frac{3}{4}, \frac{1}{4}\right), \quad b'_3 = \left(\frac{1}{4}, \frac{1}{4}, -\frac{3}{4}\right). \quad (17)$$

Each atom with mass  $M_1$  (resp.,  $M_2$ ) is linked to its four nearest neighbors having mass  $M_2$  (resp.,  $M_1$ ) by  $\Delta'$ ,  $b'_i$  (resp.,  $-\Delta'$ ,  $-b'_i$ ). Notice that

$$a'_i + b'_i = \Delta'; \quad (18)$$

see Fig. 1.

We shall now define the following discrete differences

$$D_j^+ u'_i(r'; t) \equiv v'_i(r' + \Delta'; t) - v'_i(r' + b'_j; t), \quad D_j^+ v'_i(r' + \Delta'; t) \equiv u'_i(r' + a'_j; t) - u'_i(r'; t). \quad (19)$$

The first definition can be rewritten as  $D_j^+ u'_i(r' - b'_j; t) = v'_i(r' + a'_j; t) - v'_i(r'; t)$  by using Eq. (18). Then we shall define the distortion tensor of our discrete model by a period-1 periodic function  $g(x)$  of the discrete differences

$$\begin{aligned} D_j^+ u'_i(r' - b'_j; t) &= v'_i(l + \delta_{j1}, m + \delta_{j2}, n + \delta_{j3}; t) - v'_i(l, m, n; t), \\ D_j^+ v'_i(r' + \Delta'; t) &= u'_i(l + \delta_{j1}, m + \delta_{j2}, n + \delta_{j3}; t) - u'_i(l, m, n; t), \end{aligned} \quad (20)$$

such that  $g(x) \sim x$  as  $x \rightarrow 0$ . In the continuum limit  $a \rightarrow 0$ , both discrete differences tend to the gradient of the displacement vector:

$$D_j^+ v'_i \sim \frac{\partial u'_i}{\partial x'_j}, \quad D_j^+ u'_i \sim \frac{\partial v'_i}{\partial x'_j}. \quad (21)$$

In practice, the period-1 function  $g$  should be fitted to experimental or molecular dynamics data, but it is useful to employ a piecewise linear function to illustrate the theory [7]. Notice that the displacement vectors entering the definitions (20) correspond to the lattice points closer to that on which  $D_j^+$  acts (directed along  $a_j'$ ), no matter on which fcc lattice are these points. It is important to observe that  $D_j^+ u_i'$  (resp.,  $D_j^+ v_i'$ ) is a difference between vectors  $v_i'$  (resp.,  $u_i'$ ) and it does not involve  $u_i'$  itself (resp.,  $v_i'$ ).

The potential energy of the crystal will therefore be

$$V = \frac{a^3}{4} \sum_{l,m,n} \frac{1}{8} c'_{rs pq} [g(D_s^+ u_r') + g(D_s^+ v_r')] [g(D_q^+ u_p') + g(D_q^+ v_p')]. \quad (22)$$

Here  $a^3/4$  is the volume spanned by the three primitive vectors and the additional  $1/4$  factor takes into account that both displacement vectors  $u_i'$  and  $v_i'$  yield the same displacement vector in the continuum limit. Other definitions giving different weights to  $g(D_s^+ u_r')$  and  $g(D_s^+ v_r')$  are also possible, but (22) is simple and it yields a positive potential energy.

The conservative equations of motion are

$$M_1 \frac{\partial^2 u_i'}{\partial t^2} = -T_{iq}^{-1} T_{pq}^{-1} \frac{\partial V}{\partial u_p'}. \quad (23)$$

$$M_2 \frac{\partial^2 v_i'}{\partial t^2} = -T_{iq}^{-1} T_{pq}^{-1} \frac{\partial V}{\partial v_p'}. \quad (24)$$

Using Eq. (22), these equations become

$$\frac{4M_1}{a^3} \frac{\partial^2 u_i'}{\partial t^2} = \frac{1}{4} T_{iq}^{-1} T_{pq}^{-1} \mathcal{D}_j^- \{c'_{pjrs} g'(D_j^+ v_p') [g(D_s^+ u_r') + g(D_s^+ v_r')]\}, \quad (25)$$

$$\frac{4M_2}{a^3} \frac{\partial^2 v_i'}{\partial t^2} = \frac{1}{4} T_{iq}^{-1} T_{pq}^{-1} \mathcal{D}_j^+ \{c'_{pjrs} g'(D_j^+ u_p') [g(D_s^+ u_r') + g(D_s^+ v_r')]\}, \quad (26)$$

where we have used the expressions for the standard forward and backward difference operators along the primitive directions. They are defined by  $\mathcal{D}^\pm f(R') = \pm[f(R' \pm a_j') - f(R')]$ .

To obtain the continuum limit, we add Eqs. (25) and (26), take into account the continuum limit (21), and use Eqs. (12) to revert to the dimensional orthogonal coordinates. Then the resulting equations are those of anisotropic elasticity:

$$\rho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_j} \left( c_{ijrs} \frac{\partial u_r}{\partial x_s} \right). \quad (27)$$

In this equation, the mass density  $\rho$  is the sum of the masses in the primitive cell divided by the volume thereof:

$$\rho = \frac{M_1 + M_2}{a^3/4}. \quad (28)$$

#### 4 DISLOCATIONS IN Si AND IN GaAs

Si and GaAs crystals are face-centred cubic with two atoms per lattice site, one at  $(0, 0, 0)$  and the other one at  $(1/4, 1/4, 1/4)$ . Both atoms are identical in Si (diamond structure), whereas they are different in GaAs: one atom is gallium and the other arsenic (zincblende structure). Each atom is tetrahedrally bonded to four nearest-neighbors, and the shortest lattice vector  $1/2\langle 110 \rangle$  links a second neighbor pair, as shown in Figure 2. The covalent bond between two atoms is strongly localized and directional, and this feature strongly affects the characteristics of dislocations. In turn, dislocations influence both mechanical and electrical properties of these semiconductors [3, 9]. In this Section, we shall construct dislocations for Si and GaAs.

Perfect dislocations have Burgers vectors  $(1, 1, 0)/2$  and slip on the close packed  $\{111\}$  planes. They usually lie along  $\langle 110 \rangle$  directions forming  $0$  (screw) or  $60$  (edge) degree angles with respect to the Burgers vector. Important crystallographic directions are indicated in Figure 2. The tensor of elastic constants is given by

$$c_{ijkl} = C_{12} \delta_{ij} \delta_{kl} + \frac{C_{11} - C_{12}}{2} (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + H \left( \frac{\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}}{2} - \delta_{1i} \delta_{1j} \delta_{1k} \delta_{1l} - \delta_{2i} \delta_{2j} \delta_{2k} \delta_{2l} - \delta_{3i} \delta_{3j} \delta_{3k} \delta_{3l} \right), \quad (29)$$

$$H = 2C_{44} + C_{12} - C_{11}. \quad (30)$$

in terms of the Voigt elastic stiffnesses  $C_{ij}$  and the degree of anisotropy  $H$ . Measuring temperature in degrees Kelvin and stiffnesses in units of  $10^{11}$  dyn/cm<sup>2</sup>, we have the following formulas

$$C_{11} = 16.38 - 1.2810^{-3}T, \quad C_{12} = 5.92 - 0.4810^{-3}T, \quad C_{44} = 8.17 - 0.5910^{-3}T, \quad (31)$$

for Si ( $400 < T < T_m = 873$  K) [10], and

$$C_{11} = 12.17 - 1.4410^{-3}T, \quad C_{12} = 5.46 - 0.6410^{-3}T, \quad C_{44} = 6.16 - 0.7010^{-3}T, \quad (32)$$

for GaAs ( $0 < T < T_m = 1513$  K) [11]. At 300 K,  $H$  is  $5.72 \times 10^{11}$  dyn/cm<sup>2</sup> for Si and  $5.36 \times 10^{11}$  dyn/cm<sup>2</sup> for GaAs.

To calculate the elastic far field of any stationary straight dislocation, we shall follow the method explained in Chapter 13 of Hirth and Lothe's book [9]. Firstly, we determine an orthonormal coordinate system  $e''_1, e''_2, e''_3$  with  $e''_3 = -\xi$  parallel to the dislocation line. The  $60^\circ$  perfect dislocation is directed along  $\xi = (-1, 0, 1)/\sqrt{2}$  (with a Burgers vector which is one of the primitive vectors of the lattice, and therefore glide of the dislocation leaves behind a perfect crystal [3]; see Fig. 2). We select the vector basis:

$$e''_1 = (-1, 2, -1)/\sqrt{6}, \quad e''_2 = (1, 1, 1)/\sqrt{3}, \quad e''_3 = (1, 0, -1)/\sqrt{2} = -\xi, \quad (33)$$

The Burgers vector is  $b = (0, -1, 1)/2$ . The normal to the glide plane is parallel to  $e_2''$ . In terms of the new basis, the elastic displacement field  $(u_1'', u_2'', u_3'')$  depends only on  $x_1''$  and on  $x_2''$ .

Secondly, we calculate the elastic constants in the reference system (33):

$$c_{ijkl}'' = c_{ijkl} - H \sum_{n=1}^3 (S_{in}S_{jn}S_{kn}S_{ln} - \delta_{in}\delta_{jn}\delta_{kn}\delta_{ln}). \quad (34)$$

Here the rows of the orthogonal matrix  $S = (e_1'', e_2'', e_3'')^t$  are the coordinates of the  $e_i''$ 's in the old orthonormal basis  $e_1, e_2, e_3$ . In the new reference system, the Burgers vector has coordinates  $(b_1'', b_2'', b_3'')$ .

Thirdly, the displacement vector  $(u_1'', u_2'', u_3'')$  is calculated as follows:

- Select three roots  $p_1, p_2, p_3$  with positive imaginary part out of each pair of complex conjugate roots of the polynomial  $\det[a_{ik}(p)] = 0$ ,  $a_{ik}(p) = c_{i1k1}'' + (c_{i1k2}'' + c_{i2k1}'')p + c_{i2k2}''p^2$ .
- For each  $n = 1, 2, 3$  find an eigenvector  $A_k(n)$  associated to the zero eigenvalue for the matrix  $a_{ik}(p_n)$ .
- Solve  $\text{Re}\sum_{n=1}^3 A_k(n)D(n) = b_k'', k = 1, 2, 3$  and  $\text{Re}\sum_{n=1}^3 \sum_{k=1}^3 (c_{i2k1}'' + c_{i2k2}''p_n)A_k(n)D(n) = 0, i = 1, 2, 3$  for the imaginary and real parts of  $D(1), D(2), D(3)$ .
- For  $k = 1, 2, 3, u_k'' = \text{Re}[-\frac{1}{2\pi i} \sum_{n=1}^3 A_k(n)D(n) \ln(x_1'' + p_n x_2'')]$ .

Lastly, we can calculate the displacement vector  $u_k'$  in the non-orthogonal basis  $a_i$  from  $u_k''$ .

The effect of temperature in our calculations is minimal because it enters as  $0.001T$  in Eqs. (31) and (32). A stationary perfect edge  $60^\circ$  dislocation is shown in Figure 3 for GaAs at 300 K. The corresponding dislocation for Si is similar.

## 5 CONCLUSIONS

We have proposed a model for the dynamics and statics of dislocations in face centered cubic lattices with a two-atom basis. The continuum limit of the governing equations yields the usual Cauchy equations of cubic anisotropic elasticity. Important applications of our atomic model are the Si and GaAs crystals. Similarly to the case of the linear diatomic chain in which there are acoustic and optical branches of the dispersion relation, we expect that the dynamics of the atomic model is richer than its continuum limit.

This work has been supported by the MCyT grants BFM2002-04127-C02-01 and BFM2002-04127-C02-02, and by the European Union under grant HPRN-CT-2002-00282.

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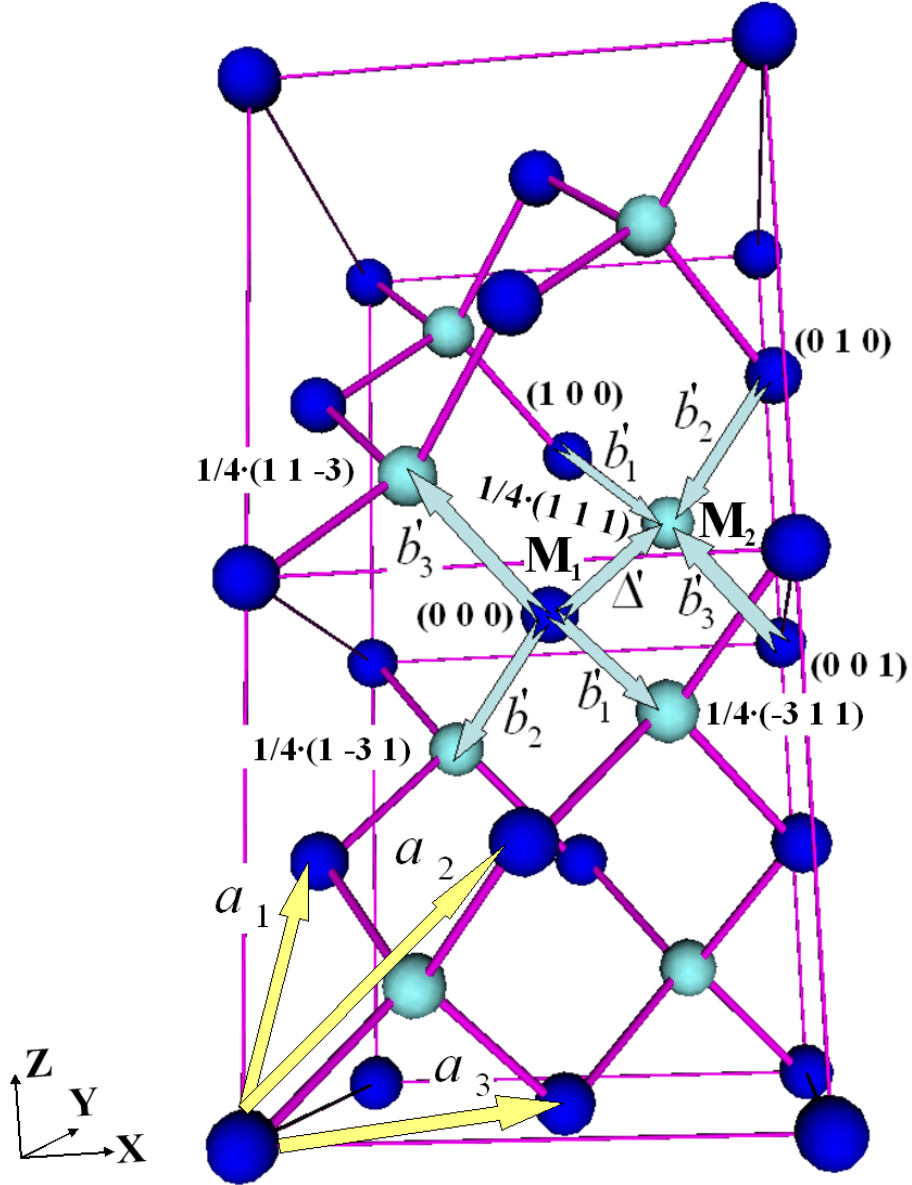


Figure 1: Relevant vectors joining lattice points that are needed to discretize the displacement field. All coordinates are expressed in the non-orthogonal basis spanned by the primitive vectors  $a_1, a_2$ , and  $a_3$ . A generic atom with position  $r' = (l, m, n)$  is placed at the origin for simplicity.

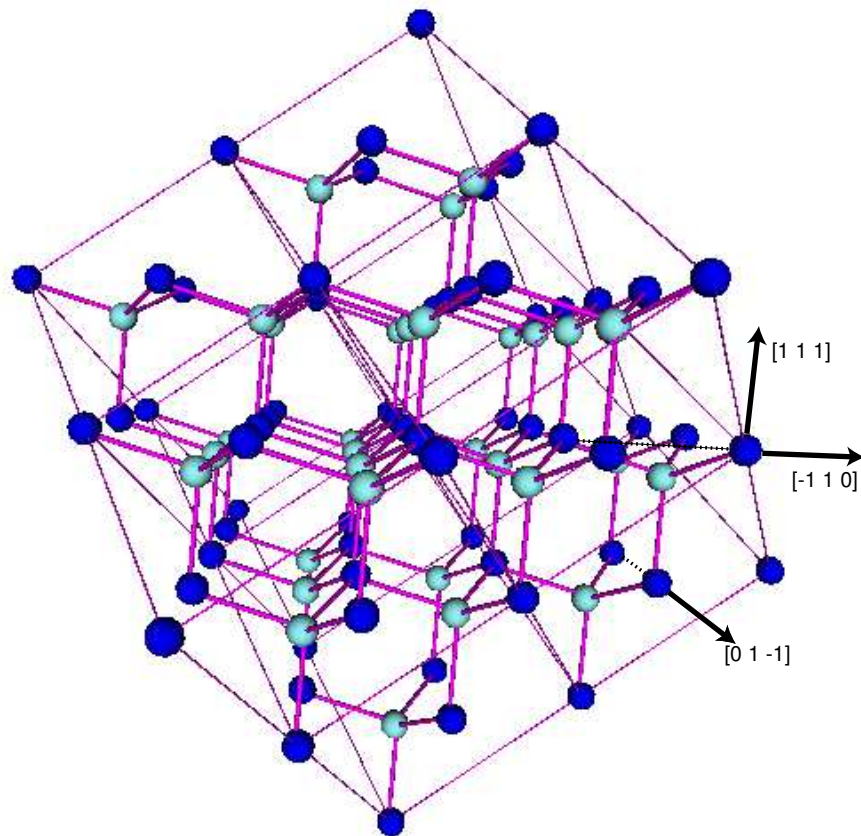


Figure 2: fcc lattice with a two-atom basis. Ga and As atoms are colored differently in the Zincblende structure and also in the diamond structure for Si, even though all atoms are identical in this case.

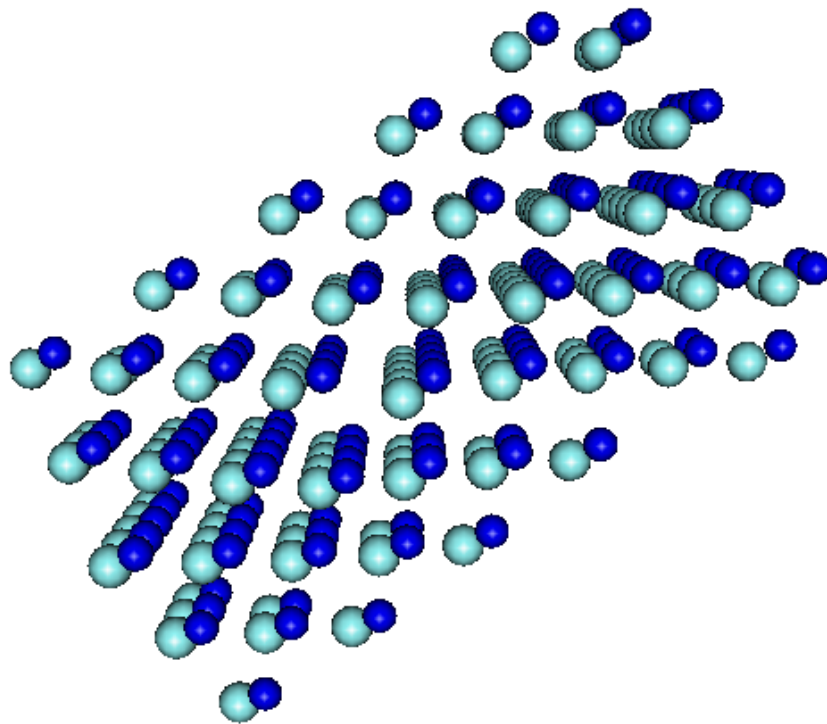


Figure 3: Perfect  $60^\circ$  dislocation in a GaAs lattice. The dislocation line is perpendicular to the paper.