OSCILLATIONS OF AN IMPURITY ATOM IN THE FIELD OF ELASTIC TENSIONS OF AN EDGE DISLOCATION

V. Gachevski†§, Hugo Aya Baquero§
†Universidad Antonio Nariño, Bogotá, Colombia, vgachevs@uniandes.edu.co
§Universidad Francisco José de Caldas, Bogotá, Colombia

ABSTRACT

Estimates were made of the energy levels and the oscillation frequencies of the impurity atom in the field of elastic tensions of the edge dislocation, based on the gradient theory of elasticity. The estimated values for the oscillation parameters of the boron atom in the silicon crystal are presented.

INTRODUCTION

The simple expressions of the gradient theory of elasticity [1] removed the singularity of the elastic tensions on the dislocations line, which exist in the classical continuum theory. Then the conception about the form of potential energy function of the interaction an atom of impurity with dislocation near the core of dislocation was changed. We carried out research into the influence of the field of tensions of the edge dislocation on the oscillations of an atom of impurity from the point of view of the gradient theory of elasticity.

DEFINITION OF THE PROBLEM

We assume that the edge dislocation is linear. The line of dislocation passes through the origin of the coordinate system coinciding with the Z-axis and the extra plane of the dislocation coincides with the half part of the YZ-plane of the coordinate system. The interaction potential of a point defect with an edge dislocation is written according to the gradient theory of elasticity as follows [2]:

$$V = b\left[-\frac{1}{r} + \frac{K_1\left(\frac{r}{\sqrt{c}}\right)}{\sqrt{c}}\right]\sin q \qquad (1)$$

where $b = \frac{mb(1+n)dv}{3p(1-n)}$, μ is the shear modulus, b is the Burgers vector, n is Poisson's ratio, dv is the volume change produced by a solute atom, K_1 is the modified Bessel function of the second kind, $\sqrt{c} = \frac{a}{4}$ and a is the lattice constant.

When the volume of the crystal is increased by the insertion of the impurity atom, then the potential (1) corresponds to the attraction of the impurity atom towards the dilatation region.

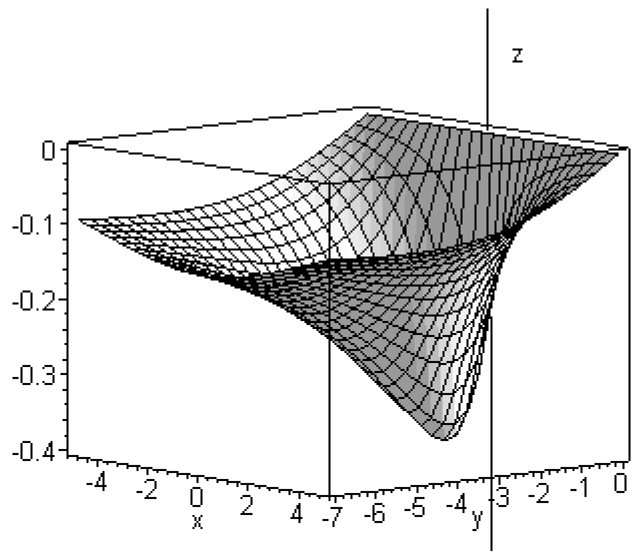

Fig. 1. Non-dimensional interaction potential function of an impurity atom with the edge dislocation in the attraction region of the atom (according to the gradient theory of elasticity) is shown.

Fig. 1 shows the potential (1) in the attraction region of the impurity through dislocation. This graph displays the minimum potential, which owing to its shape may be considered as the potential of a quantum well. The goal of our work is to estimate the frequency and the energy levels of the vibrations of the impurity atom in this quantum well.

THE SIMPLE HARMONIC OSCILLATOR APPROXIMATION

We will examine a point defect located underneath the extra plane of the edge dislocation. In this case $q = \frac{3p}{2}$ and the non-dimensional potential V^* is obtained by means of the formula

$$V^* = \frac{V\sqrt{c}}{\beta} = \frac{1}{y} - K_1(y) \qquad (2)$$

where the non-dimensional coordinate is $y = \frac{r}{\sqrt{c}}$ and r is the distance to the dislocation line.
The maximum value of the potential (2) $V^* = 0.4$ is found in the point $y_0 = 1.1144$.

The gradient theory of elasticity does not take into account the interaction between neighboring atoms but instead considers the material with the dislocation to be an elastic continuum. The impurity atom oscillates, but it cannot leave the cell of lattice due to the repulsion potential of neighboring atoms of the material. For this reason we have to add the repulsion potential of the neighboring atoms to the potential (2). Let us suppose this repulsion potential as if it were vertical walls located at the positions $y = 0$ and $y = 2\sqrt{c} + y_0$. This case corresponds to the movement of the impurity atom within a region which dimension is equal to the lattice constant a. The sum of the two potentials referred to gives a total potential which has the shape of a quantum well with vertical walls and whose bottom is given by the formula (2). Lastly, we relate this potential to a symmetric parabola $Ky^2 + by + c$. In the case of the quasi-classic approximation, we can find the frequency of the oscillations of the fundamental mode by applying the formula

$$\omega = \sqrt{\frac{K}{m}} \qquad (3)$$

where m is the mass of the impurity atom. The energy levels expression is well known and corresponds to the solution of the problem of the simple harmonic oscillator

$$E = \left(n + \frac{1}{2}\right)\hbar w \qquad (4)$$

FINAL RESULTS

The frequencies and energy levels of the oscillations of the boron atom in a silicon crystalline lattice near the edge dislocation were obtained using harmonic oscillator approximation. For this purpose, the values of the parameters of the material previously mentioned are as follows:

$\mu = 6.81\times10^{10}\ Nm^{-2}$; $b = 3.84\times10^{-9}$ m; $n = 0.218$;
$d\,v = v_B - v_{Si} = 5.05\times10^{-27}$ m^3;

When the dislocation line is in the position $y = 0$ m, the maximum value of the potential is in the position $y_0 = 1,51\times10^{-10}$ m and the depth of the quantum well is estimated at 40.1

eV, the well walls are located at the points y_l = 0 m and $\boldsymbol{y_r = 4.23\times10^{-10}}$ m. The parabolic approximation of the potential leads to the value $\boldsymbol{K = 144\,Nm^{-1}}$, where the circular frequency of the base state is $\boldsymbol{\omega = 0.895\times10^{14}\,s^{-1}}$. The energy of the base state is estimated at $E_0 = 2.95\times10^{-2}$ eV and that of the first excited state is $E_1 = 8.85\times10^{-2}$ eV. Therefore, the number of excited states within the well is N=679.

CONCLUSIONS

Upon analyzing the results of the numeric calculation, we can conclude that the energy values of the oscillations of an impurity atom near the edge dislocation may be very high. When the impurity atoms are sufficiently excited to occupy the levels of the states with the highest energy, one can expect the transition of these atoms to the base state, thus giving rise to the radiation of a photon. This effect may explain the successful functioning of the blue-light laser which was manufactured with high-density dislocation materials of the order of 10^{10} cm^{-2} [3].

REFERENCES

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