ELASTIC FIELDS AND EFFECTIVE PROPERTIES OF TRIANGULAR LATTICE WITH VACANCIES

Ekaterina Podolskaya *[1,2], Vitaly Kuzkin[1,2], Anton Krivtsov[1,2], and Mark Kachanov[2,3]

[1]*Institute for Problems in Mechanical Engineering, St. Petersburg, Russia*
[2]*Peter the Great St. Petersburg Polytechnic University, St. Petersburg, Russia*
[3]*Department of Mechanical Engineering, Tufts University, Medford, Massachusetts, USA*

Summary We consider linear elastic deformation of the two-dimensional triangular lattice with multiple vacancies. For the lattice with doubly periodic system of vacancies we derive closed-form analytical expressions for displacement field, and calculate effective elastic moduli. Molecular dynamics simulations of a lattice with random distribution of vacancies are carried out, and we compare the obtained elastic moduli with the analytical results. If the vacancy concentration is less than 4%, random and periodic distributions of vacancies produce the same effect on elastic moduli. We examine the possibilities and limitations of modeling of the lattice with vacancies by an elastic continuum with holes. We conclude that it is possible to model the effective elastic properties adequately, if the shape of the holes is chosen appropriately. Nevertheless, the strain field, in particular, strain concentration differs significantly.

The influence of point defects on physical properties of crystals is a long-standing problem in mechanics and physics of solids. Foundations of continuum theory of lattice defects have been developed in pioneering works of Eshelby [1, 2]. In continuum mechanics, such defects are modeled as pores in a homogeneous elastic medium, and continuum mechanics tools are used for calculation of displacement fields, elastic interaction of defects, effective properties of imperfect crystals, etc. Although the continuum mechanics modeling is expected to be appropriate for the effective properties, it may become inadequate at microscale, in particular, near vacancies, where the discreteness plays important role [3, 4].

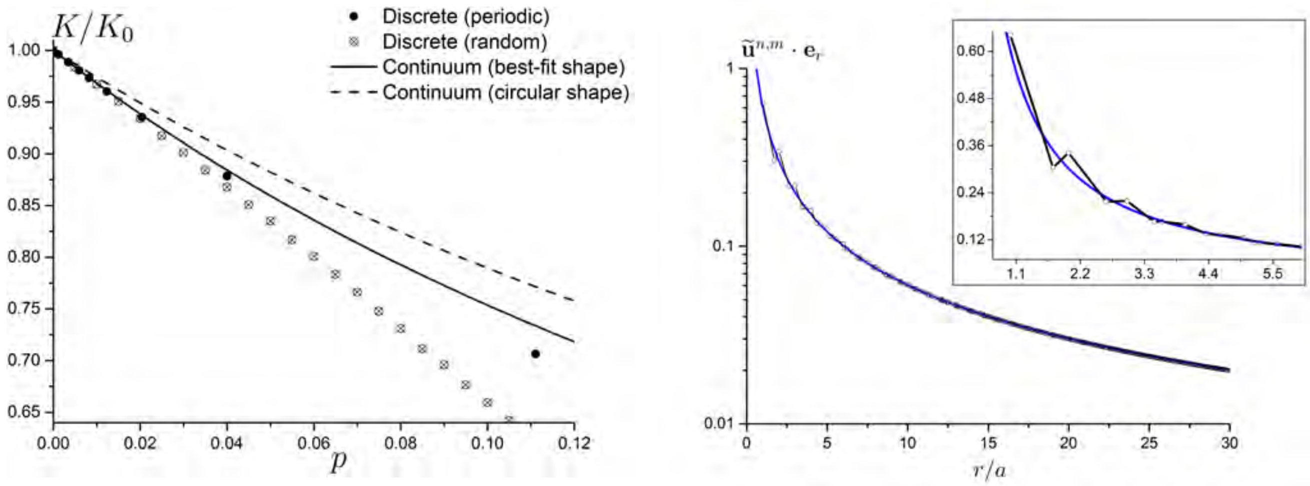
One of the first attempts to solve the problem in the discrete formulation was made by Kanzaki [5], where foundations of the so-called lattice statics method have been developed. The effect of vacancy is simulated by applying forces to atoms that simulate interatomic interactions with both the nearest and farther lying atoms. Then equations of lattice statics in harmonic approximation are solved using discrete Fourier transform. An alternative discrete approach based on lattice Green's function has been proposed by Tewary [6] who showed that this approach is equivalent to Kanzaki one, but is computationally simpler.

The two dimensional modeling taken in the present work is relevant for a variety of 2-D materials that have become available due to recent advances in technology, such as graphene, 2-D colloids, etc. Displacement fields caused by point defects in two-dimensional colloidal crystals were studied in [7, 8]. Authors have adopted Ewald summation technique for solution of continuum elasticity problems with periodic boundary conditions. It has been demonstrated that the continuum theory looses accuracy in close vicinity of defects. However, displacement fields around vacancies have not been given.

The present work focuses on elastic deformation of a triangular lattice with periodic array of vacancies. Firstly, the displacements of all particles are expressed in terms of a mean strain; secondly, using Hooke's law and defining the mean traction as the mean force acting on the cell boundary (that, in turn, is a function of displacements), the effective moduli are calculated that can be used further to find the relation between displacements and stresses applied at infinity. This approach differs from Kanzaki and lattice Green's function approaches, where the displacements are expressed in terms of interatomic forces. Note that our approach constitutes a discrete analog of doubly periodic problem in continuum elasticity [9, 10, 11]. Analytical treatment of the *discrete doubly periodic problem* is based on the exact solution of corresponding partial difference equations. Closed form expressions for particle displacements in the mentioned discrete doubly periodic problem are obtained by the use of discrete Fourier transform.

We examine the following issue: "to what extent a vacancy in triangular lattice can be modeled by a pore (hole) in elastic continuum media and what the pore shape should be?" The equivalence is considered from two points of view: (i) displacement field around a vacancy and (ii) effective elastic properties of a lattice with vacancies. Effective elastic moduli of a triangular lattice with doubly-periodic system of vacancies are calculated analytically. Afterwards, the results are compared with molecular dynamics simulations for a crystal with random distribution of vacancies. Then, the effective elastic moduli obtained in the discrete formulation are compared with prediction of continuum elasticity theory for porous medium, and the question of the pore shape is discussed. Figure 1a shows that, from the viewpoint of the effective elastic properties, a lattice with vacancies can be modeled in the framework of 2-D elasticity (plate with holes). In continuum elasticity models, the effective elastic moduli depend on pore shapes, with the circular shape being the stiffest one among all shapes of given area. However, in this case the circular pore shape assumption results in poor agreement with discrete models: the discrete system is softer. The difference between circular and best-fit shapes is even larger for the effective Poisson's ratio. Note that hole shape factors required for the best fit are substantially different from the ones for a circle, and the geometrical shape corresponding to the mentioned shape factors is not easily identifiable (and may even be non-unique).

*Corresponding author. Email: katepodolskaya@gmail.com



a *b*

Figure 1: (a) The porosity dependence of the effective bulk modulus of a triangular lattice with periodic and random distributions of vacancies. The moduli are normalized to their values in absence of vacancies. Comparison with the continuum results [12] for best-fit shape factors (solid line) and for circular pores (dashed line). (b) The radial displacement as a function of the dimensionless distance from the vacancy. Volumetric strain.

However, the strength characteristics and local fields — in particular, strain concentrations near vacancies — cannot be adequately modeled in the continuum elasticity framework. One of the crucial differences between the discrete and continuum solutions is demonstrated in the off-set figure in Figure 1b. In the vicinity of vacancy the dependence of radial component of particle displacements on distance is *non-monotonic*. In an elastic plate with a hole, the presence of the hole leads to concentration of stresses. The stress concentration factor for a circular hole under imposed volumetric strain is equal to 2 at all points of the boundary; for other shapes, the maximal, around the boundary, concentration factor is higher. Vacancy causes similar effect, however calculation of stress concentration factor is not straightforward, since stresses in discrete media are defined somewhat ambiguously [13]. We define and compute, the strain concentration factor, k, as the ratio of the maximal deformation of the bonds adjacent to the vacancy to the deformations of bonds at infinity. In the case of volumetric deformation, the maximum elongation is reached in the bonds that surround the vacancy $k_{vol} = 1.642$ that is substantially smaller than the value of 2 for the circular hole; the difference with non-circular shapes providing the best fit for the effective moduli will be larger, as well as for other modes of loading. Consider, for example, two cases of uniaxial loading along orthogonal axes x and y, with y being parallel to one of the lattice vectors. The strain concentration factors calculated using displacement field are $k_x = 1.449$ and $k_y = 1.283$ that is much smaller than the factor of 3 in the continuum Kirsch problem for a circular hole (that is even higher for non-circular shapes).

To sum up, we conclude that the effective properties of discrete media can be described by continuum theory, whereas local fields and their concentrations, specifically, strain concentration, are qualitatively different.

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