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Airy Stress Function for Atomic Models

PAUL J. STEINHARDT* AND P. CHAUDHARI

Thomas J. Watson Research Center, IBM, Yorktown Heights, New York 10598

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A simple method is shown for computing the Airy stress function for two-dimensional problems. The method is applied to a simple mechanics example and to large computer-generated atomic models whose properties are independent of some coordinate z. The method has recently proved useful for analyzing topological defects in computer-generated models of amorphous solids.

I. INTRODUCTION

For a solid in static equilibrium with cylindrical symmetry or with properties that are independent of some coordinate z, the Airy stress function provides the simplest characterization of the stress properties. For such solids, there are three independent components of the stress tensor $(\sigma_{xx}, \sigma_{yy}, \sigma_{xy})$, but all of these can be expressed as derivatives of a single scalar potential as was first noted by Airy. The Airy stress function is related to the components of the stress tensor by

$$\begin{aligned} \sigma_{xx} &= \partial^2\psi/\partial y^2; \\ \sigma_{yy} &= \partial^2\psi/\partial x^2; \\ \sigma_{xy} &= -\partial^2\psi/\partial x\,\partial y. \end{aligned} \tag{I.1}$$

For a system obeying Hooke's law and the compatibility equations, the Airy stress function, $\psi(x, y)$, in the absence of external body forces obeys a biharmonic equation

$$\Delta^4\psi(x, y) = 0. \tag{I.2}$$

By knowing the stress function, $\psi(x, y)$ for all x and y, the stress tensor field is completely specified.

If the solid is treated as a continuous medium, the Airy stress function can be found exactly in special cases where symmetries in the problem simplify the solution of the biharmonic equation (see, for example, [1]). For more complicated cases, where the medium may be inhomogeneous, solving for the Airy stress function can be a very difficult task.

* Permanent address: Lyman Laboratory of Physics, Harvard University, Cambridge, Mass. 02138.

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Of course, real solids are composed of atoms held together by interatomic forces which, in most cases, can be treated as central forces, e.g., the Lennard–Jones potential. Recently, there have been attempts to use computer-generated atomic models with central forces to analyze structural characteristics and defects in real solids [2]. When the materials are amorphous or contain defects, they are highly inhomogeneous. For cases when the properties to be studied depend only on two dimensions, the models can be treated as effectively planar and an Airy stress function can be defined. However, experience with continuum models would dictate that computing the Airy stress function for an inhomogeneous atomic model is a task too horrible to contemplate.

Surprisingly enough, this is not the case at all. The purpose of this paper is to demonstrate how one may compute for an effectively planar model composed of pins joined by rods (or atoms joined by central forces) the Airy stress function in a very efficient manner. The method applies to simple mechanics problems as well as stress properties of large atomic models. In Section II, the reasoning leading to the computation scheme will be discussed. In Section III, the notions will be demonstrated by solving a simple mechanics problem using the Airy stress function. In Section IV, the most efficient way to expand the method to large atomic models will be discussed. Several examples, ranging from stresses in finite crystalline solids to defects in amorphous solids, will be considered and the Airy stress function will be computed to determine various stress properties.

II. The Airy Stress Function in Two Dimensions

The Airy stress function was first invented in the course of analyzing stresses in continuous media and is discussed in the beginning of standard texts on the subject [1]. Because the stress function for continuous media can only be computed for cases of great symmetry, it has not received much attention as a tool for analyzing the stress properties of solids. F. C. Frank [3] was the first to note that for two-dimensional stress problems involving beams, rods, pin-joints, and the like, the Airy stress function can be easily computed and interpreted in spite of the lack of symmetry. In this section, his analysis shall be briefly reviewed.

For a two-dimensional medium, the stress is the force per unit length associated with the force necessary to hold together a cut of unit length through the medium. For a cut stretching from a chosen origin to a point x, the force necessary to keep the cut together is $F_i(x)$ and can be shown to be independent of the path of the cut. Therefore, F_i defines a force vector field and it is related to the components of the stress tensor by

$$\begin{aligned} \sigma_{xx} &= \partial F_x/\partial y; \\ \sigma_{yy} &= -\partial F_y/\partial x; \\ \sigma_{xy} &= -\partial F_y/\partial y; \\ \sigma_{yx} &= \partial F_x/\partial x. \end{aligned} \tag{II.1}$$

If one considers the shear forces on a small rectangular element in the medium with sides dx and dy, the total moment of stress (the torque) is

$$\sigma_{yx}\,dx\,dy - \sigma_{xy}\,dx\,dy. \tag{II.2}$$

In the absence of body torques, the sum must be zero or else the element would undergo a rotational acceleration. Therefore, one may conclude that

$$\sigma_{yx} - \sigma_{xy} = 0 \tag{II.3}$$

or

$$\partial F_x/\partial x + \partial F_y/\partial y = 0. \tag{II.4}$$

(Alternatively, Eq. (II.3) may have been adopted as a fundamental principle.) The last equation can be rewritten in a coordinate independent notation

$$\nabla \cdot \mathbf{F} = 0 \tag{II.5}$$

expressing the fact that the force vector field is divergenceless in the absence of body torques. The equation may be solved by introducing a continuous scalar potential which is related to the force vector field by

$$F_x = \frac{\partial \psi}{\partial y} \qquad \text{and} \qquad F_y = \frac{\partial \psi}{\partial x}. \tag{II.6}$$

Since for continuous and differentiable functions

$$\frac{\partial}{\partial x}\left(\frac{\partial \psi}{\partial y}\right) = \frac{\partial}{\partial y}\left(\frac{\partial \psi}{\partial x}\right) \tag{II.7}$$

Eq. (II.4) is automatically satisfied. Therefore, the components of the stress tensor are given by

$$\begin{aligned} \sigma_{xx} &= \partial^2\psi/\partial y^2; \\ \sigma_{yy} &= \partial^2\psi/\partial x^2; \\ \sigma_{xy} &= \sigma_{yx} = -\partial^2\psi/\partial x\,\partial y. \end{aligned} \tag{II.8}$$

For a given $F_i(x, y)$, the stress function $\psi(x, y)$ is defined up to an arbitrary constant; the physical observables are the stress and they determine the stress function only up to an arbitrary linear function in x and y.

If the two-dimensional system being considered consists of pin-joints and rods, equivalently, atoms joined by central forces, Eq. (II.8) implies that the stress function has a particularly simple form. Where there is empty space between the rods or lines of force, the stress is zero and all second derivatives of the stress function are zero. If he stress function is represented as a surface above the two-dimensional plane of the

problem with height $\psi(x, y)$ at point (x, y), in the empty spaces between lines of force the surface is flat with some constant gradient. Since the magnitude of the stress function and its gradient are not physically relevant, their value may be fixed at some arbitrary point; it is convenient to choose the value of the stress function and its gradient to be zero at some point beyond the outer boundary of the problem being considered (for problems or models of finite extent in the plane). The gradient only changes value along a line that crosses a line of force between two points. For example, if the line of force, F_x lies along the x-axis, there is an associated tension, σ_x. If a and b are points that lie on either side of the line of force on a line parallel to the y-axis, then

$$F_x = \int_a^b \sigma_{xx}\, dy = (\partial\psi/\partial y)_b - (\partial\psi/\partial y)_a. \tag{II.9}$$

(σ_{xy} is zero in the problems considered in this paper.) Thus, crossing a line of force just changes the gradient of the stress function by an amount depending on the magnitude of the force and the angle between the direction of crossing and the direction of the line of force. These rules are sufficient to determine the stress function uniquely for a two-dimensional problem.

In principle, it is possible to extend these rules to cases where there are bending moments in the problem and σ_{xy} is not equal to zero. Frank [3] has given an example of how the stress function may be computed for the case of a tensioned cross-bow. At the present time, we have been unable to extend the method to cases of covalently bonded atomic models with internal bending moments.

One might also consider extending the method to three-dimensional systems. In three-dimensions, the stress is the force per unit area and is related to the force necessary to hold together a cut surface in the medium. The forces do not form a vector field and their relation to the stress tensor components cannot be simply expressed. Also, three scalar functions[1] are necessary to determine all the components of the stress tensor. For these reasons, it is not clear how to extend the methods to three-dimensional systems.

III. Example: A Simple Mechanics Problem

Frank's intent in investigating the properties of the Airy stress function was to solve simple first-year physics mechanics problems. To illustrate the principles introduced in the previous section, a typical stress problem in elementary mechanics will be analyzed.

Problem. A car of weight W sits on the end of a cantilevered bridge as shown in Fig. 1. Determine the stresses in the supports of the bridge.

[1] The discovery that three scalar functions were necessary in three-dimensions was first made by James Clerk Maxwell.

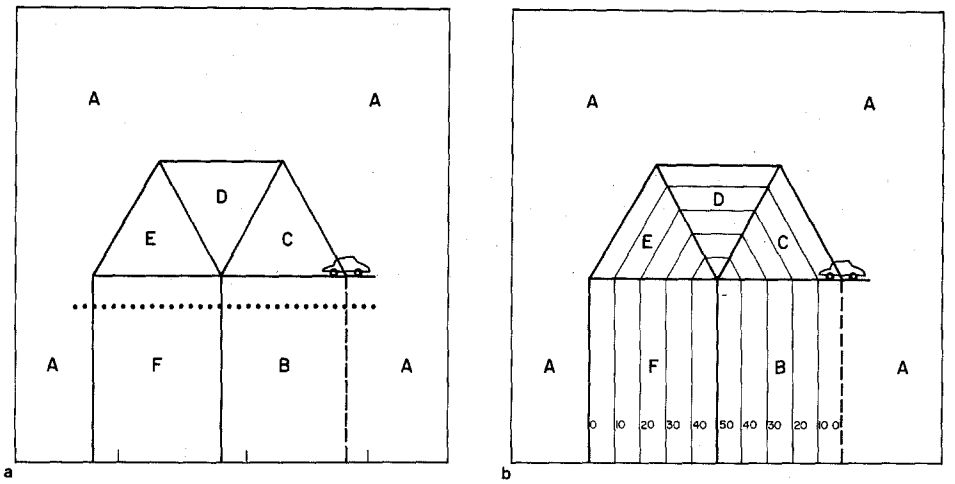

FIG. 1. A simple mechanics problem analyzed in Section III. (a) A car sits at the end of a cantilevered bridge. The car has weight W (indicated by the dotted line). (b) The contours of the Airy stress function may be easily drawn using the rules developed in Section II.

Solution. Due to gravity there is a line of force of magnitude W beginning at the car and stretching to the ground below; it has been indicated by the dashed line in Fig. 1a. In region A in the figure, the Airy stress function may be set equal to zero (actually, it can be fixed to be zero and have zero gradient at one point in region A; but since all of region A can be connected to that point by a curve that does not cross a line of force, the Airy stress function is zero everywhere in region A). The line of force due to the weight of the car can be treated just as if it were due to another strut. Therefore, one may associate a stress, σ_{yy}, along a line running from region A and B parallel on the x-axis; one finds

$$\int_a^b \sigma_{yy}\, dx = W = (\partial\psi/\partial y)_a - (\partial\psi/\partial y)_b. \tag{III.1}$$

The gradient of $\psi(x, y)$ is zero in region A and must change by an amount W as the line of force is crossed. Since the integral may be computed anywhere along the y-direction, the change in the gradient must be the same along the line of force. Therefore, the contour lines of $\psi(x, y)$ should be parallel to the line of force in region B, as shown in Fig. 1b. Because there are only pin-joints in the problem, all beams have only longitudinal compression or tension and the contour lines of the stress function must join cointinuously across them. Given the constraints in region A and the rules for changing the gradient, it is not difficult to fill in the contour lines of the stress function, as shown in Fig. 1b. To find the stresses in any member, it is sufficient to find the change in the gradient of $\psi(x, y)$ along a line running perpendicular to the member. For example, as one follows a line running from region

A–B–F–A (see dotted line in Fig. 1a) the change in the gradient along A–B must be equal to that along F–A; as a result, the change in the gradient along B–F is twice as great but of opposite sign to the other two. If the tension in A–B is W, the tension in F–A must also be W and the tension in B–F must be $-2W$. These are clearly the correct results if the structure is in static equilibrium and all forces and torques are balanced. One may proceed to analyze the stresses in the other members in a like fashion. The method is simple to apply even for rather complicated first-year physics problems.

IV. Applying the Methods to Atomic Models

The methods suggested by Frank cannot be straightforwardly applied to atomic models for two reasons. Firstly, the atomic models are three-dimensional whereas the method of computing the Airy stress function only applies to two-dimensions. Therefore, the methods can only be applied to cases where the components of the stress tensor are independent of some coordinate z. Then, since the laws of static equilibrium by which the Airy stress function is determined are vector relations, one can project atomic coordinates and forces onto the x–y plane and solve the effectively planar problem.

The second problem associated with applying the methods to atomic models is that, once the atoms and forces are projected onto the two-dimensional plane, the lines of force form a very tangled web and the regions of empty space are complex and numerous. It is therefore not practical to draw contours throughout the plane as was done for the simple mechanics problems.

The Airy stress function function may be computed for even fairly large atomic models (1000 atoms) provided that a sufficiently clever algorithm is used. We shall describe the algorithm we found to be most efficient.

Firstly, the Airy stress function is only evaluated at the intersections of a fine grid of lines that divide up the projected plane of atoms. If the grid is fine enough, there is sufficient information from knowing the Airy stress function on the discrete grid of points to analyze the stress properties of the model. If the grid lies along the x- and y-directions, one imagines integrating along the grid line beginning outside the model where the stress function is zero. As one integrates into the model, each time a line of force is crossed the gradient of the stress function is changed appropriately. The process is repeated until the integration passes once again out of the boundaries of the projected atomic model. This scheme is in fact, impractical since at each point along the integration line, each pair of interacting atoms in the model must be checked to see if the line of force joining them crosses the grid line and, if so, at what point and at what angle.

Instead, since the grid is fixed initially, one can consider each pair of interacting atoms just once and determine which grid lines are crossed by the line of force between them. Because of the linearity in the equations determining the stress function, each line of force affects the stress function independently of the others. If

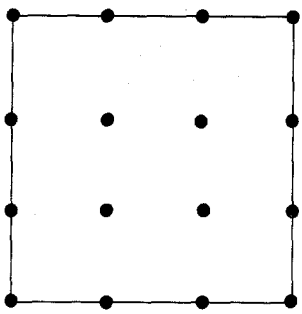

FIG. 2. Airy stress function computed for a cubic crystal of 64 atoms relaxed under a Lennard–Jones potential with cutoff equal to 1.2 times the nearest neighbor distance. Atomic positions have been superimposed.

the stress function is fixed to be zero on one end of the grid line and a line of force crosses the line at a point x', then at each point x on the other side of the intersection point the stress function is changed by an amount $F(x-x')$, where F is the component of the force perpendicular to the grid line. By repeating the computation for each grid line crossed by the line of force and for each pair of interacting atoms, one may compute the Airy stress function for a model of 1000 atoms in fractions of a minute on an IBM 370 computer.

As a test example of the method, we computed the Airy stress function for a cubic crystal of 64 atoms. The model was relaxed under a Lennard–Jones potential. For the case shown in Fig. 2 (the atomic positions have also been indicated), the potential was cut off sharply at a distance of 1.2 times the nearest neighbor distance. As a result, the Airy stress function that was found was completely trivial since each atom was able to find a position that was exactly one nearest neighbor distance from each of its neighbors. If the cutoff distance were larger, an atom would interact with its

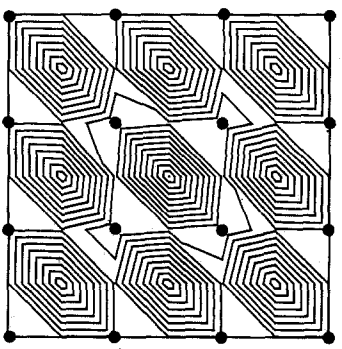

FIG. 3. Airy stress function computed for a cubic crystal of 64 atoms relaxed under an infinite range Lennard–Jones potential. Atomic positions have been superimposed.

second nearest neighbors as well as its nearest neighbors, and internal stresses in the solid would develop. In the example shown in Fig. 3, the potential was made to be infinite range, and a non-trivial Airy stress function was found. Because the interatomic force is a central force that decreases in strength with increasing distance, the stress function on each plaquette of the lattice is stretched in the diagonal direction. The second derivatives of the function contoured in the figure gives precisely the stresses one would expect from a finite crystal with infinite range interaction.

In Fig. 3, all the contours of the stress function are closed, as one would expect since the Airy stress function is set to zero everywhere outside the boundary of the model. However, in the algorithm as described above, the Airy stress function is set to zero only along one end of each grid line, i.e., along two of the four sides of the model. A powerful consistency check on the relaxation procedure is that the Airy stress function on the other boundaries is computed to have zero gradient and magnitude. If the gradient is different from zero outside the boundary, the forces (and possibly the torques) have not been balanced in the model. If the gradient is zero but the magnitude of the stress function is not, the forces are balanced but the torques are

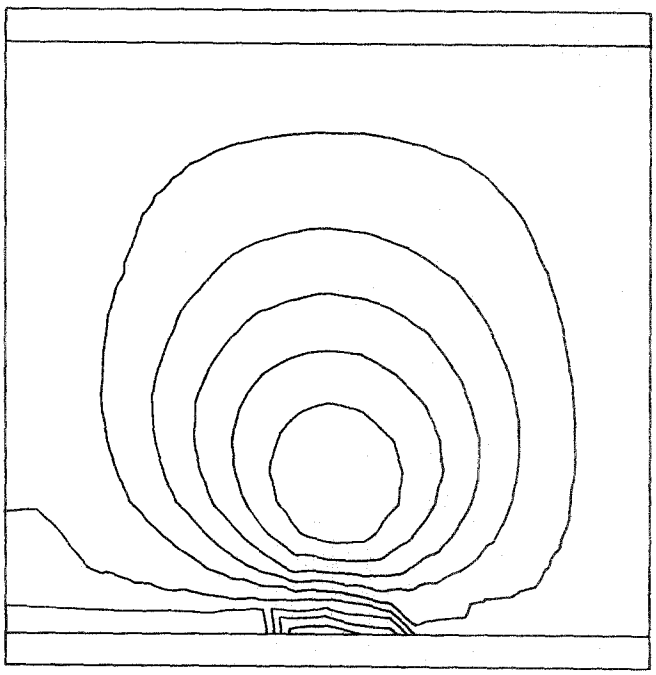

FIG. 4. Airy stress function computed for a 1000 atom fcc crystal relaxed under Lennard–Jones potential cutoff at 2.1 times the nearest neighbor distance. Three atoms have been fixed in the relaxation. As a result, the forces are not truly equilibrated and the contour lines of the stress functions do not close. The region of greatest peaks is where the three fixed atoms lie in the model.

not. As an example of how sensitive the consistency condition is, consider Fig. 4. Figure 4 represents the Airy stress function found for a 100 atom fcc crystal after many relaxations of the model under a cutoff Lennard–Jones potential. The relaxation procedure normally holds three atoms fixed in the model during the relaxation to eliminate net rotations and translations of the model. As a result, the forces between the fixed atoms and their neighbors are never quite equilibrated. Even though the three atoms (which are usually chosen to lie near one another in the model) represent a small percentage of the total number of atoms in the model, they have a tremendous impact on the computation of the Airy stress function. As one can observe in Fig. 4, the Airy stress function is highly perturbed around a small region near the boundary where the three atoms lie. In fact, the contour lines of the stress function stretch beyond the boundary of the problem and do not close. The only remedy to this that we found was to relax the model many times fixing different sets of three atoms until the contour lines of the stress function did close. (See Figs. 5 and 6.) However, the example demonstrates how the computation of the stress function can be used to verify the success of a relaxation procedure.

The method of computing the Airy stress function has been usefully applied in an attempt to analyze dislocations in amorphous solids. A dislocation is a line defect which, in a crystal, can be detected by comparing the Burger's circuit (the line integral of the displacement) in the dislocated crystal to that in an undislocated crystal. The dislocation leads to non-trivial stresses which, if the line defect lies along the z-axis, are independent of z. The Airy stress function may therefore be defined, and, for an edge dislocation in a continuous medium, the Airy stress function may be determined exactly [1],

$$\psi(x, y) \propto y \ln(x^2 + y^2). \tag{IV.1}$$

However, in an amorphous solid, one cannot possibly see if the solid contains a defect since there is no reference lattice with wwhich one can compare Burger's

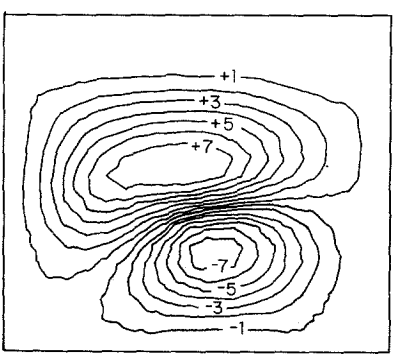

FIG. 5. Airy stress function computed for 1 1000 atom fcc crystal with an edge dislocation relaxed under Lennard–Jones forces with a cutoff of 2.1 times the nearest neighbor distance. The dislocation has not been perfectly centered and finite boundary effects can be observed.

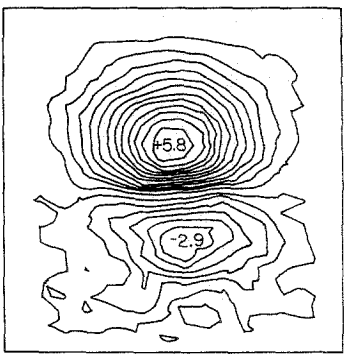

FIG. 6. Airy stress function computed for a 4000 atom amorphous solid with a dislocation relaxed under a Lennard–Jones potential cutoff at 1.2 times the nearest neighbor distance.

circuits. On the other hand, if and amorphous solid can be shown to have an Airy stress function characteristic of a dislocated crystalline solid, one may conclude the amorphous solid also contains a dislocation.

Therefore, a dislocation was first placed in a perfect fcc crystal by cutting away a half plane of atoms and relaxing the remaining atom under Lennard–Jones potential. The Airy stress function was computed for a model relaxed under a Lennard–Jones potential cut off at 2.1 times the nearest neighbor distance and the result shown in Fig. 5 was found. The results are consistent with Eq. (VI.1) once it is realized that the model is of finite extent and the dislocation has not been placed precisely in the center of the model.

When the same procedure was followed for an amorphous solid composed of over 4000 atoms, the results shown in Fig. 6 were found. We found that the Airy stress function of the dislocated amorphous solid is very similar to a dislocated and relaxed crystalline model, although with a smaller maximum value for the stress function in the amorphous solid compared to the crystalline. From this one may conclude that dislocations, or at least localized entities with characteristics very similar to dislocations, can be stabilized in amorphous solids under static relaxation.

V. CONCLUSIONS

Because the Airy stress function is a single function that contains all the information about the stresses within an effectively planar solid, computing the Airy stress function is the most convenient way of determining the stress properties of the solid. Because the stress function in continuous media is usually difficult to determine, the stress function has seldom been considered as a practical tool.

Building on the suggestions of Frank, we have shown that even for rather large atomic models with central forces the Airy stress function can be computed in a very efficient scheme. We have demonstrated that it may serve to sensitively test whether a

solid has been equilibrated under the interatomic forces and may aid in determining structural properties of the solid. Thus, it would be recommended to those investigating stress properties in problems ranging from simple mechanics to solid state physics that they refamiliarize themselves with the very useful Airy stress function and its interpretations.

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