Archives of Mechanics • Archiwum Mechaniki Stosowanej • 29, 3, pp. 365—375 Warszawa 1977

A continuum model of the dislocation core

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A CONTINUUM model, which includes higher strain gradients in the constitutive equations, is shown to be the equivalent of a periodic array of discrete dislocations. The particular problem that is considered is the Taylor model of the dislocation core. However the approach is general and any other model could be used. The continuum model can be made as accurate as one wants by taking a sufficient number of terms. Thirteen gradients are sufficient to model the core to a specified (reasonable) accuracy. In the Appendix a theory which includes only three gradients is evaluated in terms of a common model of the glide process.

Wykazano, że model ośrodka ciągłego, zawierający w równaniach konstytutywnych wyższe gradienty odkształcenia, jest równoważny periodycznemu rozmieszczeniu dyskretnych dyslokacji. Problem szczególny, jaki tu jest rozważany, stanowi model Taylora ośrodka dyslokacyjnego. Rozwiązanie nasze jednakże jest ogólne i również każdy inny model może być zastosowany z powodzeniem. Model kontynualny może być dowolnie dokładny, wystarczy tylko uwzględnić odpowiednią liczbę wyrazów. Trzynaście gradientów wystarcza do modelowania ośrodka z żądaną (rozsądną) dokładnością. Zamieszczona w Dodatku teoria zawierająca tylko trzy gradienty została wyznaczona za pomocą prostego modelu procesu poślizgu.

Доказано, что модель сплошной среды, содержащая в определяющих уравнениях высшие градиенты деформации, эквивалентна периодическому распределению дискретных дислокаций. Частная задача, которая здесь рассматривается, составляет модель Тейлора дислокационной среды. Наш подход однако является общим и каждая другая модель может быть с успехом применена. Континуальную модель можно сделать так точной, как требуется, достаточно только учитывать соответствующее количество членов. Тринадцать градиентов достаточно для моделирования среды с требуемой (разумной) точностью. Помещенная в дополнении теория, содержащая только три градиента, определена при помощи простой модели процесса скольжения.

1. Introduction

THE concept of a dislocation as an excess (shortage) row of atoms inserted into an otherwise perfect array can be relatively easily understood at the atomic level. In the past this writer has had great difficulty in understanding the connections that have been proposed for relating these atomic dislocations and the macroscopic level observations of plastic deformations. The need for a continuing action process is evaluated by HEAD [1]. Many attempts at providing the connections are not clear on what is assumed, on what is predicted and what could come from combining some elementary dimensional analysis with the experimental data. Especially hard for an outsider to fathom are the *limitations* of the specific models.

Experimental data on many metals indicate the 95% of the plastic work appears as heat while 5% goes into the "stored energy" of cold work. The heat more or less corresponds to the dissipation in the core of the dislocation and the storage of energy to the elastic energy in the "far field". Calculations concerning the far field are based on the

continuum view of matter and indeed even assume a reversible elastic material. These far field calculations, taken as a class, are quite successful and very useful in leading to increased understanding of some concepts of macro-level plasticity. They suffice, for example, in a discussion of how dislocations interact with each other or with other defects.

There are major problems when considering the core region and in metals that means with 95% of the energy. A discussion of the more successful core models is given in HIRTH and LOTHE, [5, p. 217f].

To construct a continuous model of nature which contains every detail of the atomic model, we visualize replacing the discrete variables by continuous ones in the same sense that the density function is the analogue of the discrete masses. Once a perfect continuous model exists, there still remains the question of *how to simplify* it to the point where it would be practical for stress analysis work. For any given approximation to the perfect continuous model, one can then ask, what continuum framework assumptions must be made in order to produce the same results. Clearly the perfect atomic model does not exist so that imperfect ones must be considered.

The writers view of a good connection between the discrete model and the corresponding continuous one is given by MINDLIN [6] concerning polarization.

The Taylor dislocation potential is the atomic model to be considered here. To permit a complete and systematic connection to be made between the atomic model and the continuum one, the Taylor potential is replaced by its Fourier series representation. We then develop a one dimensional continuum theory which produces the same stresses as the Taylor model, *including those in the core region.*

As anticipated, the continuum theory so developed is quite complex, and is based on some non-classical concepts. It is also very specialized and is possibly not the most efficient continuum model of the real dislocation. Nevertheless, it is complete, involves tight assumptions and provides whatever accuracy one needs. The basic steps in the formulation of the continuum theory were given by DILLON *et al.* [1–3]. The basic concepts are the use of generalized stresses which depend on higher spatial gradients of the strain. The net result of such a theory is a local and very nonhomogeneous spatial deformation field in problems which classically have a homogeneous strain. Thus an accurate continuum theory which is the complete counterpart of the Taylor atomic-level model is created. It is extremely important to the writer that the reason one normally develops strain gradient theories is to include non-local effects. For if one fact characterizes the atomic level properties of a dislocation, it is that its very presence affects its distant neighbors.

DILLON *et al.* [1–3] were formally complete but it was not clear there how to select the particular deformation gradients which should be used. The present paper illustrates the procedure for deciding on the number of gradients needed in a continuum theory when one assumes the Taylor model of a dislocation is valid.

It is customary in atomic models to use interatomic potentials φ and then to calculate "stresses" as $d\varphi/dx$. On the other hand, continuum theories of the type utilized below are easier to *motivate* by using *deformation gradients.* Stresses are then calculated from the associated constitutive equations. Thus the quantitative connection between the two models of matter is made via their respective stresses, whereas much of the paper will directly involve either potentials or deformation gradients.

Potentials with certain properties are created from descriptive data. An overall governing theory of the potential does not seem to be commonly used. Thus Frenkel assumed that the perfect part of matter in one dimension was

$$\varphi = -\frac{b}{2\pi} A \cos \frac{2\pi x}{b}, \tag{1.1}$$

where b is the interatomic spacing and x is the generic coordinate. The stresses associated with this potential are

$$\sigma = A \sin \frac{2\pi x}{b}. \tag{1.2}$$

The parameter A is identified with the ideal strength of the material. For small strains it can be evaluated in terms of the elastic modulus. However, the maximum stress in (1.2) is much greater than the values that one usually observes. Hence imperfections must be considered.

The continuum theory of the "potential" in the perfect material has to be governed by

$$\Phi'' + \left(\frac{2\pi}{b}\right)^2 \Phi = 0, \tag{1.3}$$

where primes denote derivatives with respect to x.

2. The Taylor model

By introducing (deleting) an extra row of atoms whose effect could extend several atoms, Taylor developed the potential near the core of the dislocation to be

$$\varphi = -A \cos 2\pi \frac{x}{\lambda}\left(\frac{N+1}{N+\frac{1}{2}}\right) - A \cos 2\pi \frac{x}{\lambda}\left(\frac{N}{N+\frac{1}{2}}\right), \tag{2.1}$$

where λ and N are core width and the number of atoms in the core, respectively when the external force vanishes. Dislocations which are located at a uniform spacing l are assumed. We therefore rewrite the potential equation (2.1) in its Fourier components

$$\varphi = -\frac{bA}{2\pi} \cos \frac{2\pi x}{b} + \sum_1^\infty A_n \sin \frac{n\pi x}{l} + \sum_1^\infty B_n \cos \frac{n\pi x}{l}. \tag{2.2}$$

The stresses associated with this potential are therefore

$$\sigma = \frac{d\varphi}{dx} = A \sin \frac{2\pi x}{b} + \sum_1^\infty \frac{n\pi}{l} A_n \cos\left(\frac{n\pi x}{l}\right) - \sum_1^\infty \frac{n\pi}{l} B_n \sin\left(\frac{n\pi x}{l}\right). \tag{2.3}$$

Thus the Fourier representation equation (2.2) of the Taylor model of the dislocation is taken here as *the* dislocation model that should be equivalent to the continuum theory that is to be developed. Obviously, if other dislocation models are chosen, the details will be different but the concept for developing the continuum counterpart remains the

same. The numerical results given below show that the significant frequency components of equation (2.2) lie in a relatively narrow band and that within that band, none of them can comfortably be neglected. Thus we shall say that φ is adequately(1) approximated by

$$\varphi = -\frac{bA}{2\pi}\cos\left(\frac{2\pi x}{b}\right) + \sum_{N}^{M} A_n \sin\left(\frac{n\pi x}{l}\right) + \sum_{N}^{M} B_n \cos\left(\frac{n\pi x}{l}\right). \tag{2.4}$$

Table 1. Fourier Series Coefficients for the Eq. (2.4) minus the "far field"

14	1.074691×10^{-2}	-6.776649×10^{-2}
15	-3.173898×10^{-2}	-7.665861×10^{-2}
16	-7.819515×10^{-2}	-5.682711×10^{-2}
17	-10.83353×10^{-2}	-0.853763×10^{-2}
18	-10.51785×10^{-2}	5.357944×10^{-2}
19	-6.479734×10^{-2}	10.57196×10^{-2}
20	$-0.0011196 \times 10^{-2}$	12.60481×10^{-2}
21	6.479263×10^{-2}	10.57586×10^{-2}
22	10.52436×10^{-2}	5.36406×10^{-2}
23	10.85202×10^{-2}	-0.852533×10^{-2}
24	7.848066×10^{-2}	-5.70000×10^{-2}
25	3.196807×10^{-2}	-7.713532×10^{-2}
26	-1.083497×10^{-2}	-6.851721×10^{-2}

The stresses obtained from the Eq. (2.4) are than

$$\sigma = A\sin\left(\frac{2\pi x}{b}\right) + \sum_{M}^{N} A_n\left(\frac{n\pi}{l}\right)\cos\frac{n\pi x}{l} - B_n\left(\frac{n\pi}{l}\right)\sin\frac{n\pi x}{l}. \tag{2.5}$$

Thus the continuum theory which leads to stresses given by the Eq. (2.5) will be the continuum analogue of the discrete dislocation theory. Therefore, the criteria for selecting gradients which should be included in the continuum theory, and which was absent in Dillon has been developed. Namely, it must be a theory whose "stresses" contain those frequencies contained in the Eq. (2.5). By adjusting coefficients it will be shown below that the stresses can be made identical in both theories.

3. Continuum model

We temporarily set aside considerations of the atomic potential and discuss higher gradient elasticity theories which have become popular in some circles in recent years. For illustrative purposes, we limit to linear elastic theories and assume that equilibrium exists. We also consider that one-dimensional theories suffice for illustrative purposes and assume certain formal material parameters are zero. We first illustrate a continuum theory which contains the far field stresses given by the Eq. (1.1).

(1) This is where one uses the idea of how accurate an approximation one needs.

One-dimensional classical elasticity is governed by $\partial\Sigma/\partial x = 0$ and the constitutive equation $\Sigma = E\frac{\partial u}{\partial x}$. When these are combined the displacement equations are. Hence the solution is

$$E\frac{\partial^2 u}{\partial x^2} = 0, \quad u = A + Bx.$$

The constants A and B are evaluated for each particular problem by specifying boundary conditions. They cannot be matched to the stresses, the Eq. (1.2), and classical theory is inadequate for matching to the atomic model except for small strains.

The new type materials are also governed by an equilibrium equation of the form

$$\frac{\partial \Sigma}{\partial x} = 0, \tag{3.1}$$

but the constitutive equations([2]) contain higher deformation gradients such as

$$\Sigma = E\frac{\partial u}{\partial x} + F_2\frac{\partial^3 u}{\partial x^3}. \tag{3.2}$$

The displacement equations are obtained by combining equations (3.1) and (3.2) to be

$$E\frac{\partial^2 u}{\partial x^2} + F_2\frac{\partial^4 u}{\partial x^4} = 0. \tag{3.3}$$

Thus the displacement is

$$u = A + Bx + \frac{c}{\beta}\sin\beta x - \frac{D}{\beta}\cos\beta x, \tag{3.4}$$

where

$$\beta = \left(\frac{E}{F_2}\right)^{\frac{1}{2}} \tag{3.5}$$

and A, B, C and D are arbitrary constants.

Thus the frequency β is formally determined by material constants in (3.1) and (3.2) which are analogous to the elastic modulus E. Suppose (for convenience) that one chooses the origin so that $c = 0$. Then the stress is

$$\Sigma = B + D\sin\beta x \tag{3.6}$$

and we have the classical term represented by *B and in addition an oscillatory one.* By adjusting (i.e. interpreting) the material constants the second term in (3.6) can be made to match the "far field" stress in the Eq. (2.2) which is associated with the potential equation (2.1). In other words the far field fixes F_2 in the Eq. (3.2). In particular if

$$F_2 = \frac{Eb^2}{4\pi^2} \tag{3.7}$$

and D is the ideal material strength, the stresses in the continuum model (3.6) exactly coincide with those in the atomic field equation (2.2) when the external force vanishes

([2]) The Eq. (3.2) is chosen for simplicity and neglects some interaction.

(making $B = 0$). In most continuum problems there simply is no need to simultaneously consider the residual stresses associated with the periodic atoms and those due to external loads and therefore in practice we have developed the habit of considering each separately.

The procedure is quite similar in principle if one wants to establish the continuum theory which has the stress field associated with the dislocations which are uniformly spaced. The materials are governed by equilibrium equations of this form:

$$\frac{\partial \Sigma}{\partial x} = 0 \tag{3.8}$$

and the newer constitutive equations (but still very special ones) are assumed to be

$$\Sigma = E\frac{\partial u}{\partial x} + F_2\frac{\partial^3 u}{\partial x^3} + F_3\frac{\partial^5 u}{\partial x^5} + \ldots F_p\frac{\partial^n u}{\partial x^n}. \tag{3.9}$$

The displacement equations then become

$$E\frac{\partial^2 u}{\partial x^2} + F_2\frac{\partial^4 u}{\partial x^4} + F_3\frac{\partial^6 u}{\partial x^6} + \ldots F_p\frac{\partial^{2p} u}{\partial x^{2p}} = 0. \tag{3.10}$$

Since this is a linear d.e. with constant coefficients the solution is routine. While perhaps cumbersome to relate to the specific material constants F_p, the solution of the Eq. (3.10) can be expressed as

$$u = A + Bx + \frac{\bar{c}_1}{\beta_1}\sin\beta_1 x + \frac{\bar{c}_2}{\beta_2}\sin\beta_2 x + \ldots \frac{\bar{c}_p}{\beta_p}\sin\beta_p x - \frac{\bar{D}_1}{\beta_1}\cos\beta_1 x - \frac{\bar{D}_2}{\beta_2}\cos\beta_2 x - \ldots \frac{\bar{D}_p}{\beta_p}\cos\beta_p x. \tag{3.11}$$

Hence the stresses are obtained from the Eqs. (3.9) and (3.11) to be

$$\Sigma = B + c_1\cos\beta_1 x + c_2\cos\beta_2 x + \ldots c_p\cos\beta_p x + D_1\sin\beta_1 x + D_2\sin\beta_2 x + \ldots D_p\sin\beta_p x. \tag{3.12}$$

Thus if we associate the far field with the β_1 frequency, we need to have $p-2 = N-M$ in order that the stresses (3.12) be *identical* with those in (2.5).

In order that the stresses of (2.5) and (3.12) match, the coefficients of (2.5) and (3.12) must coincide. In the formal solutions of continuum problems these coefficients $c_1 - c_p$ and $D_1 - D_p$ are determined by boundary conditions. It is possibly going to be difficult to prescribe the boundary values of the appropriate gradients. Nevertheless this procedure illustrates how to develop a possible continuum theory *with all of the atomic-level detail retained.* It will be shown below that the same frequency band suffices when one applies an external force to the atomic model. The coefficients change but no additional terms are needed in the model.

In books on dislocations one frequently sees pictures of the "glide" (slip) process where one block of atoms is displaced relative to another. The dislocation is important to the mechanism but not to end result which is a purely kinematic situation where atoms initially in a line have moved to a new location. One might wonder if a continuum model could represent this way of considering dislocations. The answer is yes, as illustrated in the Appendix where the *displacements* are used for connecting the two different models.

4. Numerical results

We have computed the Fourier series coefficients and associated frequencies for the representation of a potential consisting of a perfect lattice, except in the core region where the Taylor potential, the Eq. (2.4), is used. We next considered different truncations of the complete series, in order to simplify the corresponding continuum model. Typical

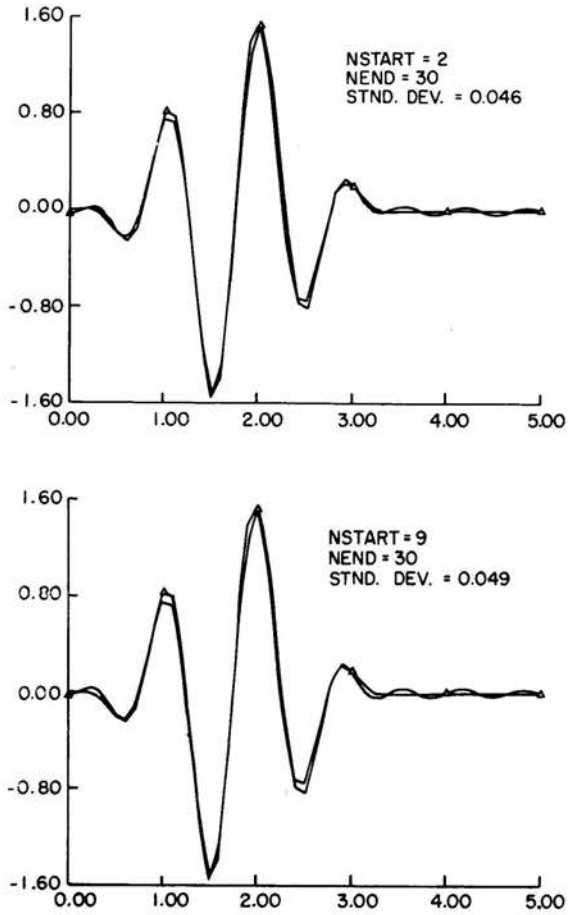

FIG. 1. (Upper) A comparison of the Eq. (2.4) minus the far field with a truncated Fourier series beginning at $N = 2$ and ending at $N = 30$. (Lower) The same as above except starting at $N = 9$.

results are shown in Fig. 1 where the exact potential is compared with a truncated one consisting of 29 different frequencies.

Since the Taylor model itself is schematic, we considered also somewhat cruder fits where larger standard deviations for the difference between the exact and the approximate one were obtained. For example, the results shown in Fig. 2 were obtained([3]) with con-

([3]) The results in Figs. 1 and 2 were obtained by simply neglecting the remainder of the series. A better fit could be obtained by adjusting some of the coefficients.

siderably fewer terms than those of Fig. 1. As a matter of personal judgement, we consider the case $N = 14$ and $M = 26$, shown in Fig. 2, to be an adequate approximation to the Taylor model. The Fourier series coefficients for this case are shown in Table 1.

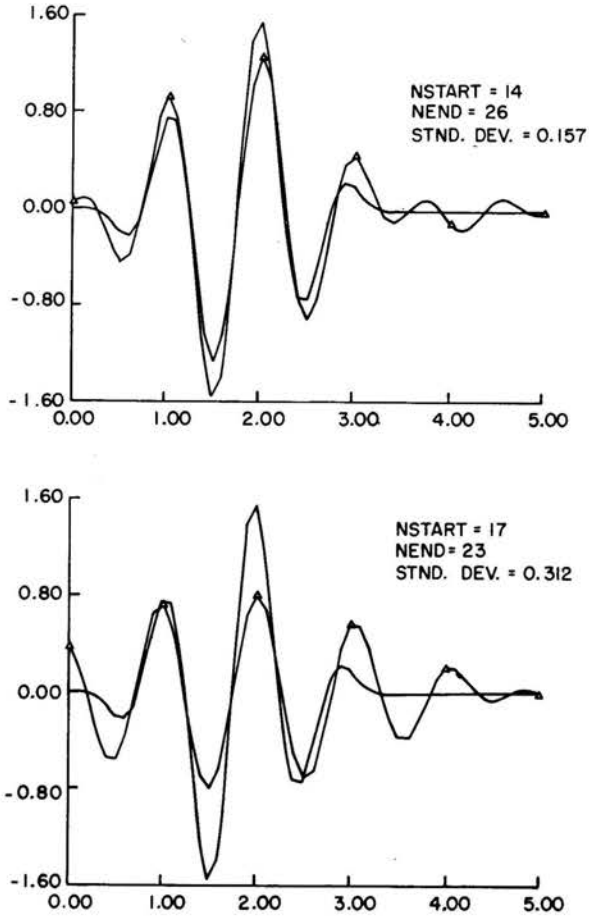

FIG. 2. (Upper) The same as Fig. 1, except starting at $N = 14$ and ending at $N = 26$. (Lower) The same as Fig. 1, except starting at $N = 17$ and ending at $N = 23$.

5. External force

When an external force is applied to the discrete model the Taylor potential in the core region is

$$\Phi = -A\cos 2\pi\frac{(x-\delta)}{\lambda}\left(\frac{N+1}{N+\frac{1}{2}}\right) - A\cos 2\pi\frac{x}{\lambda}\left(\frac{N}{N+\frac{1}{2}}\right). \tag{5.1}$$

The shape of this potential was calculated by Taylor and is used to describe how the dislocation core "moves" under the action of an applied force. We have also computed the coefficients for the Fourier representation of a potential consisting of a perfect lattice except for the core where the Eq. (5.1) applies. The results obtained indicate that precisely the *same frequencies* are needed for the Eq. (5.1) as for the Eq. (2.4). The magnitudes of the coefficients change but the frequencies do not.

Thus by *selecting the number of gradients p according to the relation* $p-2 = N-M$, one obtains a *continuum stress* Σ which is precisely the same as the *stress* σ calculated from the truncated Fourier series of the discrete model potential.

6. Discussion

We have demonstrated above how one can develop a continuum model which has the properties usually associated with a discrete picture of nature including the core of the dislocation. The particular atomic model is due to Taylor, but it is clear that any other one could have been used as well.

A number of factors have been left out in order to more clearly make the main point. For example, dislocations are used to explain work hardening through their interactions. Considerations of certain points becoming "unpinned" are not investigated. Furthermore, one clearly needs a constitutive equation that is different from the Eq. (3.2) if one wants the dislocation to stay in its new location when the external load is removed. These and many other aspects of dislocations can be considered but they obviously depend on this begin the process for developing the continuum model.

It is our fond hope that the results given in the Appendix will become accepted by continuum workers and that the viewpoint presented there will enhance mutual collaboration between them and metallurgists. A continuum theory with two or three strain gradients in it should prove tractable and at the same time provide sufficient "structure" to retain the main features of dislocation core phenomena. It is doubted that one can make much practical use of the more complete theory. Certain specialized features may become useful but the complete picture is too complex. Said differently, the writer sees very little hope of having sufficient boundary data in the near future which can be used to specify a unique theory with thirty gradients in it.

Appendix 1

The core properties of a dislocation are important in understanding the mechanism of plastic deformation. On the other hand, suppose one wants to consider a process where the core is included but the precise details are not so important. On might think, is the situation as complicated as that given above?

Consider the "glide" (slip) process where one block of atoms is permanently displaced relative to another. There may be some merit in comparing the atom positions before plastic deformations occured with their locations afterwards. While this is an *incomplete*

picture, it is a useful calculation. The most frequent picture of this process in shown in Fig. 3. We consider that the glide planes are spaced $L_0 = 2$ units apart and that the relative displacement is given by PL_0. Thus we have a *purely kinematic* picture to consider. Therefore we attempt to match *displacements* between the models rather than stresses as above. The macroscopic plastic strain P in this process is

$$P = \delta/h. \tag{A.1}$$

The relative motion of the atoms can be represented by a continuous function $U(x_2)$. Hence, we represent the difference between the actual and average displacements by a Fourier series

$$U(x_2) - Px_2 = \sum_{n=1}^{N} A_n \sin\frac{n\pi x_2}{h} + \sum_{n=1}^{N} B_n \cos\frac{n\pi x_2}{h}. \tag{A.2}$$

Clearly the number of terms required in the representation depends on the specific atomic model, i.e. $U_1(x_2)$. If the displacement actually occurs as suddenly as frequently indicated,

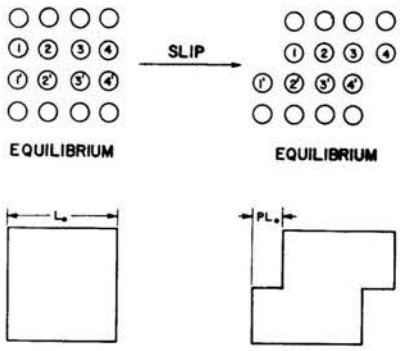

FIG. 3. A schematic picture of "glide".

a large number of terms will be required in (A.2). However, many other writers [2] "smooth out" the transition region so that it occurs over several atomic planes. Thus if one does not insist on too precise a fit, the results shown below indicate that *two or three Fourier frequencies* suffice to represent the nonhomogeneous strain field associated with the core. Since the atomistic displacements are usually not well known anyhow, these are judged to be reasonable fits. Given this fact, then one can construct a simpler gradient theory. The procedure is the same as that used above but the material parameters have a very different physical interpretation. However a theory with three gradients can do a remarkably good job of approximating the small scale nonhomogeneous deformations which are an inherent part of plastic deformations.

Since most uses of the discrete atomic model are schematic rather than explicit, this representation may be closer to the view of most investigators who use electron microscopes than is the Taylor model.

Results for retaining terms from $N = 1$ to $N = 4$ are shown in Fig. 4. It is our judgement that the case $N = 3$ is adequate for modeling nature. That is, the Fourier series with three terms is as close to "reality" as the curve it is representing.

This indicates that a continuum theory which incorporates higher deformation gradients in its constitutive equations can be considered to be a continuum analogue of the discrete atomic model of glide. Furthermore two or three Fourier series terms do a fairly decent job of providing some core region structure and that in turn means a continuum theory which considers only two or three higher gradients.

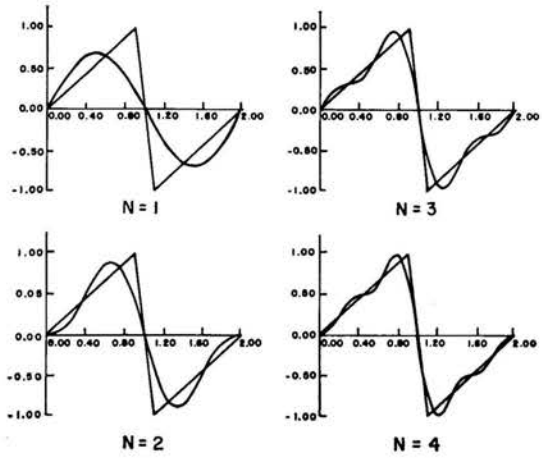

FIG. 4. A comparison of the Eq. (A.2) with a truncated Fourier series, beginning at $N = 1$ and ending with $N = 1, 2, 3,$ and 4 as indicated.

References

1. O. W. DILLON, jr. and P. PERZYNA, *A gradient theory of materials*, Arch. Mech. Stos., **24**, 5–6, 727–747, 1972.
2. O. W. DILLON, jr., *Continuum thermoplasticity and dislocations*, in: Inelastic Behavior of Solids, (ed. by KANNINEN, ADLER, ROSENFIELD and JAFFEE), McGraw-Hill, New York 1970.
3. O. W. DILLON, jr. and J. KRATOCHVIL, *A strain gradient theory of plasticity*, Intl. J. Sols. and Structs., **6**, 12, 1513–1533, 1970.
4. A. K. HEAD, *Dislocation theories of the plastic properties of metals and the transition to continuum mechanics*, in: Inelastic Behavior of Solids (ed. by KANNINEN, ADLER, ROSENFIELD and JAFFEE), McGraw-Hill, New York 1970.
5. J. P. HIRTH and J. LOTHE, *Theory of dislocations*, McGraw-Hill, New York 1967.
6. R. D. MINDLIN, *Continuum and lattice theories of dielectric films*, Intl. J. Sols. and Structs., **5**, 11, 1197–1208, 1969.
7. G. I. TAYLOR, *Mechanism of plastic deformations of crystals* I, Proc. Roy, Soc. A., **145**, 362–387, 1934.

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Received March 28, 1975.