Early Work on Imperfections in Crystals, and Forerunners of Dislocation Theory

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Early work on imperfections in crystals, and forerunners of dislocation theory

By A. K. Seeger

In his 1913 contribution to the *Encyclopädie der mathematischen Wissenschaften* entitled 'Physikalische Grundlagen der Festigkeitslehre', written in collaboration with L. Föppl, T. v. Kármán[1] reviewed the processes resulting in the permanent deformation of crystalline materials, i.e. twinning ('einfache Schiebung') and glide ('Translation'), from the molecular point of view ('Raumgitterhypothese'). In the last chapter, v. Kármán treats the phenomena of mechanical hysteresis and mechanical aftereffects in crystals and crystalline aggregates. He states clearly that in 'homogeneous' crystals (in modern language, in perfect crystals) dissipation of mechanical energy is possible only through the processes resulting in heat conduction but that the existence of 'Trennungsflächen' may lead to mechanical hysteresis and, in connection with thermal fluctuation, to aftereffects and hence to internal friction other than that associated with heat conductivity. This thinking, which from the modern viewpoint must be considered as essentially correct if we understand by 'Trennungsflächen' not only grain boundaries but any extended perturbation of the ideal crystal structure,† was mainly based on a molecular model proposed by Prandtl but not published until 1928.[2]

In his 1928 paper, Prandtl reiterated that a perfect crystal ('störungsfreier Kristall') would give rise neither to mechanical hysteresis nor to mechanical aftereffects and that hence grain boundaries or subgrain boundaries ('Verwachsungsstellen einzelner Kristallite') and defects inside the crystals ('Störungen des regelmäßigen Gitteraufbaus im Innern') must be held responsible for these phenomena. He also pointed out that defects inside the crystals must be quite frequent after plastic deformation. For both types of imperfections, Prandtl[2] proposed the following 'Gedankenmodell', which in his opinion retained most of the essential features of the physical situation: molecules situated between two perfect crystalline regions possess a direction of easy displacement. They are elastically bound to equilibrium positions relative to one of the crystallites. In addition to this they are subject to a spatially varying force resulting from the other crystallite and incommensurate with respect to the force field exerted by the first crystal. Prandtl showed that in the absence of thermal fluctuations this model permits permanent deformations, corresponding to metastable states, and devoted most of his paper to a fairly detailed treatment of the time-dependent phenomena possible in this model because of thermal fluctuations.

† v. Kármán[1] recognized the importance of 'metastable equilibrium states' in solids that are retained as a result of the cooling of crystals from high temperatures and the suppression of the approach to equilibrium at low temperatures.

Prandtl's model, which according to v. Kármán[1] dates from 1913 or before, is presumably the first atomistic model of a crystal imperfection. From a historical point of view it is interesting to note that by 1928 at the latest Prandtl[2] had a rather clear picture of the merits and limitations of his model. For instance, in full agreement with the present view he recognized that the phenomenon of work-hardening required a three-dimensional treatment of the crystal imperfections and that it could not be accounted for in a physically satisfactory way by his one-dimensional model. He also discussed the implications of his 'Gedankenmodell' for recovery and recrystallization and emphasized that it might be a useful starting point for a model of friction and wear.

Essentially independently but acknowledging the equivalence of his basic assumptions with those of Prandtl, U. Dehlinger[3] arrived at virtually the same model in his 'Habilitationsschrift'. Dehlinger recognized that a plastically deformed metal consists mainly of regions which are only slightly deformed but that there must be localized perturbations which extend to some degree into the less deformed parts of the crystals. He called them 'Verhakungen' and proposed that their dissolution ('Auflösung') upon heating is the basic recrystallization mechan ism of deformed metals. In contrast to Prandtl,[2] who handled the deformation aspects of the model mainly by means of geometrical analogies, Dehlinger gave a full theoretical treatment. Since Dehlinger's treatment is basic to much of the later work, I shall here give a brief outline of it.

The boundary atoms of the 'bottom' crystallite (figure 1) experience a potential energy, exerted by the 'top' crystallite, of the form

$$\Phi = A \sin^2 \pi y_n, \tag{1}$$

where y_n is the displacement of the individual atoms measured in units of the lattice spacing b in the glide direction. The force constants between neighbouring atoms is denoted by α. The conditions of equilibrium then read

$$\partial\Phi/\partial y_n - \alpha b(y_{n-1} - 2y_n + y_{n+1}) = 0 \tag{2a}$$

or

$$(\pi A/b) \sin 2\pi y_n - \alpha(y_{n-1} - 2y_n + y_{n+1}) = 0 \quad (n = \ldots, -2, -1, 0, +1, +2, \ldots). \tag{2b}$$

Modifying Frenkel's[4] estimate of the theoretical shear strength of a crystal slightly, Dehlinger[3] found, for f.c.c. metals with slip direction $\langle 110 \rangle$,

$$A = \tfrac{\sqrt{3}}{4}\pi^{-2} G/b, \tag{3}$$

where G is the shear modulus in the glide system. He related the constant α to the Young modulus and obtained

$$\alpha = (2\pi^2 A/b)(1+\mu), \tag{4}$$

where μ denotes the Poisson constant.

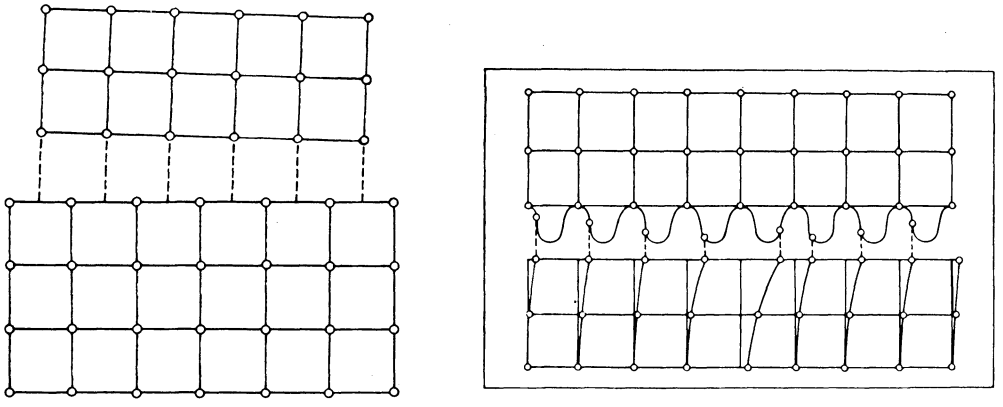

FIGURE 1. Dehlinger's[3] model of a 'Verhakung' (in modern language, two closely spaced dislocations of opposite sign).

Dehlinger[3] treated the case of a strongly localized 'Verhakung' (figure 1) by assuming that ($2b$) may be linearized for $|n| \geqslant 2$ and demonstrated that it would presumably not be stable. He went on to show that stability may be achieved if a situation is considered in which the two crystallites are displaced with respect to each other over sufficiently large distances (in his words: 'Reihe von Verhakungen derselben Richtung').

J. Frenkel & T. Kontorova[5] considered the same model but were interested mainly in its dynamical aspects. They generalized ($2b$) to

$$m\frac{\mathrm{d}^2y_n}{\mathrm{d}t^2} = -\frac{\pi A}{b}\sin 2\pi y_n + \alpha(y_{n-1}+y_{n+1}-2y_n), \tag{5}$$

where m is the mass of the atoms. Frenkel & Kontorova[5] looked for solutions of the form

$$y_n(t) = y_{n+1}(t+\tau) \tag{6}$$

propagating with a speed

$$w = b/\tau. \tag{7}$$

Assuming that terms higher than second order in the Taylor expansion in powers of τ may be disregarded, they arrived at the ordinary differential equation

$$m'\,\mathrm{d}^2y_n/\mathrm{d}t^2 = -(\pi A/b)\sin 2\pi y_n, \tag{8a}$$

with

$$m' = m-\alpha\tau^2. \tag{8b}$$

With linearization of the right-hand side, ($8a$) describes the usual small-amplitude oscillations for $m' > 0$. Frenkel & Kontorova[5] showed that, for $m' < 0$, ($8a$) admits the solution†

$$y_n = 2\pi^{-1}\arctan\left[C_0\exp\{(\pi/b)\sqrt{(-A/m')}(t-n\tau)\}\right], \tag{9}$$

† The condition $m' < 0$ means that the velocity w of propagation of (9) is always less than the sound velocity $w_0 = b\sqrt{(\alpha/m)}$ of the model.

where C_0 is a constant of integration, and stated: 'This case corresponds to an elementary slipping of the atomic chain, constituting the phenomenon of slip propagation.' They mentioned that this slipping motion may be compared to Taylor's 'dislocations'.[6] In view of the general knowledge reached at the time it is surprising that Frenkel & Kontorova[5] stressed that 'such "dislocations" are only a result and not the cause of slip process' and that according to their views 'slipping can take place in a perfectly ideal crystal lattice without any "dislocations" in the sense of Taylor's theory'. They mention that solutions analogous to (9) may be used to describe the twinning of crystals.

Dehlinger & Kochendörfer[7] discuss Frenkel & Kontorova's solution (9) in considerable detail and emphasize that in their opinion it does represent the 'dislocations' described by Taylor[6] and J. M. Burgers[8]. They consider the application to chain reactions in crystals ('Kettenreaktionen') such as the allotropic transformation of cobalt and martensite formation. They coined the expression 'Eigenbewegungen' ('characteristic motions') for 'aperiodic atom movements propagating through the entire lattice' and proposed that standing waves of finite amplitude with macroscopic wavelength should be possible, too. In their opinion such standing waves might result from the reflection of solutions such as (9) at grain boundaries.

In the summer of 1948 U. Dehlinger & A. Kochendörfer suggested to me to attempt as 'Diplomarbeit' a generalization of the Frenkel–Kontorova solution (9) to dislocation propagation between two lattice planes with slightly different spacings. In the course of this work it was quickly realized that Frenkel & Kontorova's method for arriving at a tractable differential equation such as (8a) was highly special and not suited for the treatment of general dynamical problems. In a search for a more general approach the discrete displacements $y_n(t)$ were replaced by a continuous variable $y(n, t)$, and the approximation

$$y_{n+1}(t) - y_n(t) \approx \partial y(n, t)/\partial n \tag{10}$$

was made. From the Lagrangian of the Prandtl–Dehlinger–Frenkel–Kontorova model and Hamilton's variational principle the Euler–Lagrange equation

$$\alpha \frac{\partial^2 y}{\partial n^2} - m \frac{\partial^2 y}{\partial t^2} = A \sin 2\pi y_n \tag{11}$$

was obtained.† It appears that this was the first time that the equation now widely named 'sine-Gordon equation' was written down in a *physical* context. Not very much later and independently, F. C. Frank & J. H. van der Merwe[11] arrived at (11) by essentially the same reasoning. However, (11) is much older and had been very thoroughly studied in the context of differential geometry[12]. This formed the starting point for the work of Seeger *et al.*[13] on the time-dependent solutions of (11).

† Some of the results were later published in a joint paper with A. Kochendörfer.[10]

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