CHAPTER 1

The Mechanics–Materials Linkage

MARC A. MEYERS
University of California, San Diego
RONALD W. ARMSTRONG
University of Maryland
HELMUT O. K. KIRCHNER
University of Paris

1.1 HISTORY

Mechanics is a much older discipline than materials science. Several books, Todhunter and Pearson [1], Love [2], Truesdell [3], Timoshenko [4], and an encyclopedia article [5], give historical sketches. Briefly, solid mechanics started in the seventeenth century with the mathematical analysis of Galileo, followed soon after by Hooke, the Bernoullis and Euler, who derived differential equations of beams under various equilibrium conditions. The material properties were of concern only through constants in the differential equations and, otherwise, received little attention. Hooke's law, published as an anagram, introduced the concept of an elastic modulus. Much later, Cauchy coupled more closely the determination of material constants with the concepts of stress and strain and introduced the consideration of anisotropic elastic constants. Worry about material defects and their influences in mechanics started with da Vinci's observation that long ropes are more likely to break than short ones if subjected to the same loads. Advances in mechanics, then, as now, were closely connected with developments in mathematics, in particular, with the origins of differential and integral calculus, that occurred in the seventeenth and eighteenth centuries.

Materials science, that is, study of the relationship between the properties of materials and their internal structures, is a twentieth-century outgrowth of met-

Mechanics and Materials: Fundamentals and Linkages
Edited by Marc A. Meyers, Ronald W. Armstrong, and Helmut Kirchner
ISBN 0-471-24317-5

allurgy (one of the oldest metallurgical texts is the 1556 book "De Re Metallica" by Agricola). The subject took hold during World War II and was introduced as an academic discipline within universities in the postwar years, for example, following on from such pioneering textbooks as authored by Seitz [6], *Physics of Metals* and Barrett, *Structure of Metals* [6a]. Sufficient advances in chemistry, physics, mathematics, and mechanics aspects of materials properties, constitutions, and internal structures had occurred during the war to provide a new curriculum. Orowan [7] pointed out at the time that much progress had been made after the turn of the century (late 1890s–early 1900s), when Otto Mohr, of Mohr circle fame, ascribed too many variables within the internal structure of materials to allow scientific investigation of such structural influences on mechanical properties. Quickly the newborn subject widened from metallurgical concerns with steel to aircraft and nuclear alloys, then, from metals to ceramics, rocks, concrete, composites, and, recently to cellular, biological, and biomimetic materials.

The relatively late development of materials science as a discipline was intimately connected with the dearth of characterization tools to enable quantitative observations of the internal structures of materials at the level that mattered, now extended with modern instrumentation past the microstructural scale to nanostructures. Beginning from origins in optical metallography, the embryonic discipline of materials science received great impetus in the 1920s from quantitative X-ray diffracted intensity measurements that showed, through match with theoretical model calculations, most materials to be structurally imperfect on the crystal lattice scale. These observations were followed in the 1950s by X-ray diffraction imaging (X-ray topography), field ion emission, and, particularly, transmission electron microscopy (TEM) studies that provided direct observations of defect structures at high magnifications.

1.2 MODERN TOOLS

1.2.1 Modern Materials Science Tools

From the earliest investigations of materials, the dimensional scale of observations and processed material particle sizes have decreased from centimeters to angstroms, encompassing a range in spatial resolution of nine orders of magnitude. Perhaps the greatest impact of instrumentation was made by the obtainment of TEM images of dislocations in thin foil metal samples, as first reported by Hirsch and colleagues [8] and Bollmann [9] in the 1950s. The possibility of observing internal microstructures within materials on a submicrometer scale led to better understanding of known material behaviors and validated even earlier theoretical model descriptions of crystal dislocation properties. For example, the preeminent question of whether grain boundaries were regions of amorphous layers or were essentially crystalline was soon resolved via field ion and electron microscopy in favor of crystallinity at atomic dimensions.

Currently, bright-field and dark-field electron microscopy provide ongoing assistance with understanding the structural nature of increasingly complex materials, for example, as demonstrated by the direct observation of charge density waves. It is, however, fair to say that mechanics-based investigations able to make use of the most recently acquired knowledge are rare. An exception is the quantitative analysis of internal stress distributions pioneered by Mughrabi [10]. Now atom probe and electron microscopy are performed on the atomistic level accompanied by strain measurements and chemical analysis on that same level. Elegant surface-layer observations and localized chemical analyses via atomic excitations or scattering mechanisms are accomplished more or less routinely with the scanning electron microscope (SEM). The technique has revolutionized mechanics-related fractographic studies where comparisons of fracture surfaces may be made with archival results to identify sources of failure and consequent failure mechanisms. A recent accomplishment is to section at a micrometer scale isolated cleavage regions on an essentially ductile fracture surface so as to reveal the underlying particle-associated microstructural causes for the transition from ductile fracturing to cleavage [11].

Modern diffraction techniques are providing great insight into material constitutions and lattice perfections. Historically, the first identifications of "invisible phases" were accomplished with X-ray diffraction by Guinier [12] and Preston [13]. Current examples are the use of sophisticated neutron diffraction to investigate sintering phenomena [14] and small-angle scattering and positron annihilation for analysis of precipitation [15]. These are instances where experimental techniques and theoretical analyses have used a common language: both description of the experimental techniques and their interpretations via Khachaturyan's theory [16] move easily through reciprocal space. Whenever complementary experimental techniques are combined, there is synergy. Hardening mechanisms in quite sophisticated industrial alloys have been identified by neutron diffraction and electron microscopy [17]. Classical X-ray work has been upgraded to a new level by employing synchrotron radiation and charge couple devices or image plates as detectors. The development of high-energy (1-MeV) electron microscopes with commensurate higher resolution (0.12 nm) has brought the scale of observation down to individual atoms.* Now, the positions of individual atoms in a grain boundary and grain boundary structural transformations are observed. Analytical (high-resolution) electron microscopy (AEM) has become a reality.

Electron microscopy, since its discovery by Ruska in 1932 [18], and field ion microscopy (see Cerezo et al. [19]) have undergone dramatic changes in recent years. Image processing and analysis are accomplished through the explosion of computer availability and advanced computational methods. An entire universe of micro- and nanoconstituents and defects has been identified and mapped past the first observations of dislocations. Two chapters in this volume are dedicated

*On October 27, 1998, S. J. Pennycook (Oak Ridge National Laboratory) showed ⟨110⟩ silicon images with a resolution of 0.08 nm.

to this topic: Chapter 5, by Thomas, and Chapter 9, by Veyssière. Some of the techniques are listed below:

Position-sensitive atom probe (POSAP) (spatial resolution at 0.2–0.3 nm)
High-resolution electron microscopy (HREM) (spatial resolution ~0.3 nm)
Convergent beam diffraction (CBD) (spatial resolution 20 nm)
Energy dispersive X-ray spectroscopy (EDS) (spectral resolution at 50 nm)
Electron energy-loss spectroscopy (EELS) (~100 nm resolution)
Atom location by channeling enhanced microanalysis (ALCHEMI)
Scanning transmission electron microscopy (STEM)
Energy loss near edge spectroscopy (ELNES)
Subelectron volt subangstrom electron microscopy (SESAME)
Auger electron spectroscopy (AES): for probing surfaces.

The list of new methods of characterization, already developed or under development in the past 10 years, has considerably enhanced the capability of materials scientists and mechanicians to probe into the very appreciable depths of materials. Recent ongoing Materials Research Society (MRS) symposia have been dedicated solely to specimen preparation, thus providing direct demonstrations of such importance. Considerable time may be spent on the preparation of a single successful specimen. Some of the more recent additions to the arsenal of sample preparation techniques are

Ultramicrotomy
Lapping machines
Electron-beam lithography
Computerized ion milling

Beyond the obtainment of careful experimental observations of defects is their match with computer simulations of the defect appearances, thus reinforcing positive identifications. Figure 1.1 illustrates the synergism between electron microscopy and computer modeling. A stacking fault in a TiAl specimen can only be incontrovertibly characterized if its image (Fig. 1.1*a*) is compared with computer-generated images. By assuming different atomic configurations and imaging conditions, different images are obtained in the computer simulation. The correct image is the one that most closely resembles the actual micrograph.

Figure 1.2 illustrates how high-resolution TEM can detect very small structural changes, which may, potentially, have a dramatic effect on mechanical properties. Whereas Figure 1.2*a* shows a clean tilt boundary in Mo, Figure 1.2*b* shows the boundary with a 1.5 nm layer of body-centered tetragonal carbide. This distortion changes the atomic configuration of the boundary in a significant manner. The reader should verify this by setting the paper at an angle and seeing how the straight lines "curve" at the boundary.

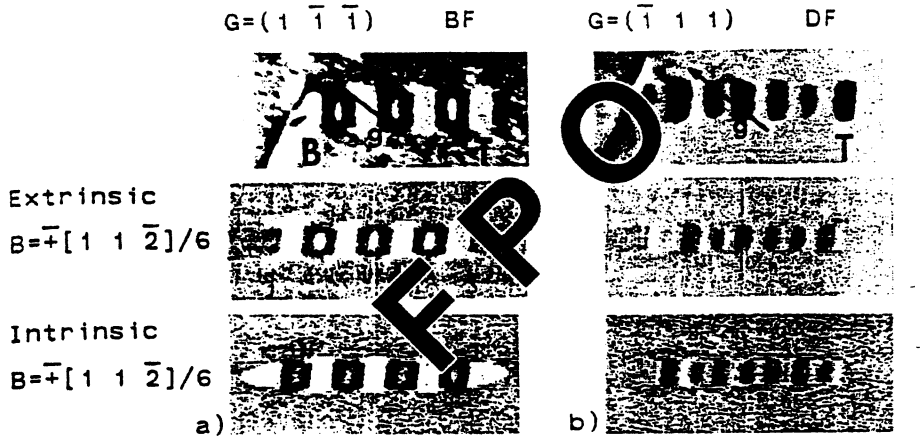


Figure 1.1 Experimentally observed (top) (by TEM) and computed contrast (middle and bottom) for faulted dipole in TiAl. [From G. Hug, A. Loiseau, and A. Lasalmonie. *Phil. Mag. A* **54** (1986), 47, Fig. 6, p. 55.]

Interfaces pose a great challenge for mechanicians and materials scientists and constitute a new frontier of research. The mechanical performance of materials is deeply affected by their interfaces, and minute quantities of foreign atoms, concentrated at these interfaces, can completely alter their toughness. In composites and the microelectronic industry, especially, interfaces play a crucial role.

1.2.2 Modern Mechanics Tools

Despite its advanced age, the discipline of mechanics experienced a similar explosive development over the same period described for the primal development of the subject of materials science. The rapid development and availability of computers provided for transition from difficult analytical techniques to implementation of problem-solving "codes" that could hardly have been imagined even a decade ago. The mechanics of structures, extending from the largest scale (geomechanics, aircraft, bridges, sailing boats) to microscale systems (thin films and graded materials), and, now, to the electromechanics of biological molecules, all rely on numerical computations. Before computers became available, mechanics was largely restricted to analytical methods based on advanced mathematical techniques, or, at best, employment of time-consuming numerical methods. The rapid growth of numerical capabilities, and their diminishing cost, first allowed straightforward but cumbersome numerical calculations to be undertaken, leading to the replacement of differential equations by difference equations in finite element techniques, and, finally, the direct simulation of the mechanical situation, with possible incorporation of Monte Carlo or molecular dynamics methodologies.

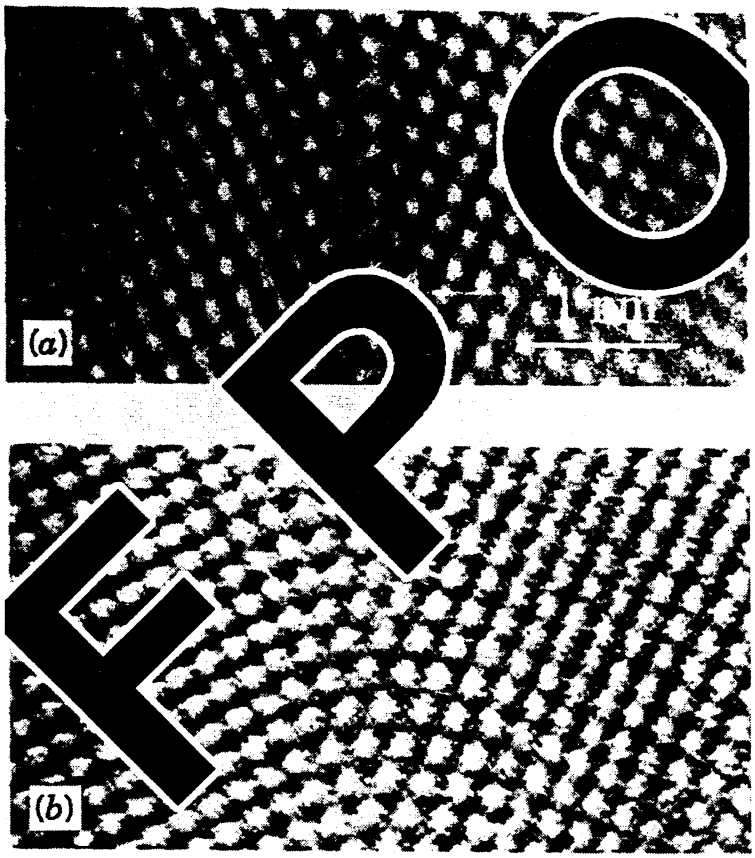
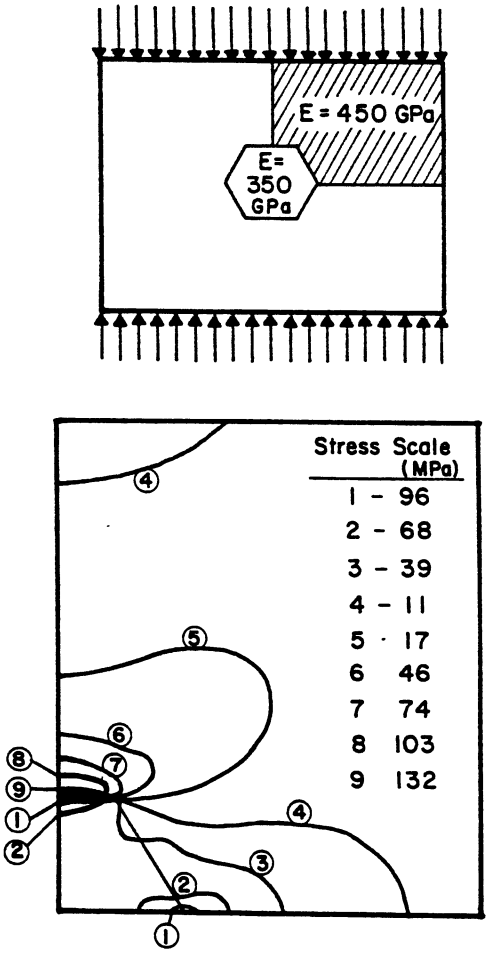


Figure 1.2 High resolution electron micrograph of a 37.1° tilt boundary in molybdenum. The tilt axis is [001], the boundary plane (310). (*a*) The boundary in pure material, no carbon or oxygen detectable by Auger spectroscopy. (*b*) The boundary after carburization containing a 1.5 nm wide layer of body centered tetragonal carbide. (Courtesy of J.-M. Penisson, CEA, Grenoble.)

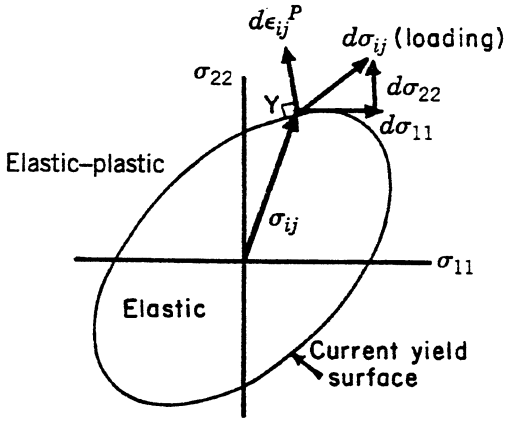
Already, commercial finite-element programs that have been tailored to mechanics studies, such as ABACUS, ADINA, ANSYS, EPIC, KATIA, and MARC, and that are fully user-friendly, are available for mechanics and materials applications, analogously to the situation for word processing programs that are currently in service. Such tools, which are employed at this time mainly for obtaining serious computational mechanics solutions, will become commonplace in the mechanics–materials domain. This is demonstrated for the subject area of anisotropic elasticity by Barnett in Chapter 4. The analysis developed by Stroh, once considered to have only special application, because of the necessity to solve a sextic equation, is now used rather routinely, for example, by "electronic chip" developers confronted with thermal stress problems in multilayer structures. An example of application involving heterogeneity on a two-



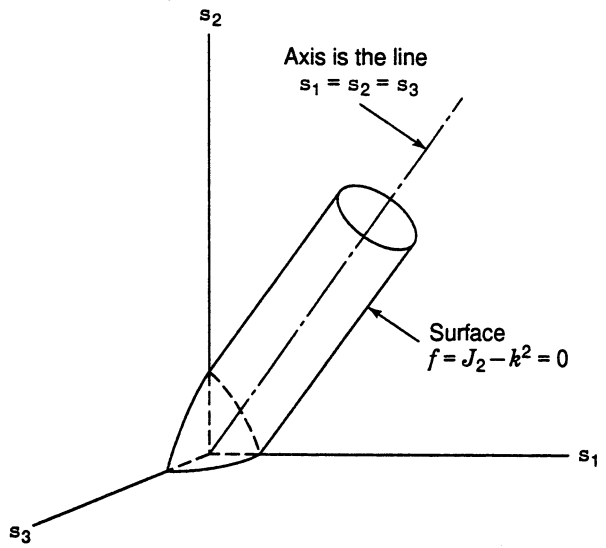
Ed: Dashes from 5-9 are missing. Add (a) & (b).

Figure 1.3 Compliant hexagonal inclusion in a stiff matrix subjected to compressive stresses created by uniaxial compressive loading, (a) schematic of problem and quarter spaced hatched (loading traction of 1 GPa); (b) finite-element computation with isostress lines σ_{11} indicated. (From D. A. Hoke, M. A. Meyers, and G. T. Gray, unpublished results.)

dimensional scale is shown in Figure 1.3 for a compliant hexagonal inclusion that modifies the isotropic stress field of a compressed specimen. The calculation was done with the MARC code employing MENTAT pre- and postprocessors (automatic meshing) on a Sun (Sun Microsystems, Inc.) workstation. One half day was required for program setup and problem solution. The indicated stress fields were readily obtained. An applied compressive stress of 1000 MPa (1GPa) was shown to generate orthogonal stresses (perpendicular to the loading direction) between −96 and +132 MPa. Thus, compressive tractions can gener-



(*a*)



(*b*)

Figure 1.4 (*a*) Two-dimensional representation of yielding (von Mises); (*b*) three-dimensional representation of yield surface.

ate tensile stresses in anisotropic polycrystals. Three-dimensional solutions are already accessible.

An example of analytical developments in mechanics that are finding their way into the materials world are the concepts outlined below. Plastic flow is often simplified as a one-dimensional (unidirectional) process in materials science studies, where stress and strain are essentially taken to be scalar quantities.

The shape of the stress–strain curve is determined by dislocation motion, and slip takes place in the direction and plane of maximum resolved shear stress (according to the Schmid law). A continuum mechanics viewpoint would be to add consideration of the same phenomenon in three-dimensional space, leading to the concept of a yield surface determining the boundary in all directions between elastic and plastic deformation. An ellipse is delineated in a two-dimensional plane containing the principal stresses, as defined by the J_2 yield criterion of von Mises (see Fig. 1.4*a*). The ellipse is obtained as the intersection of a cylindrical yield surface with an inclined plane (see Fig. 1.3*b*). The second invariant (J_2) of the deviatoric stress tensor given by the definition:

$$J_2 = \tfrac{1}{2}\sigma'_{ij}\sigma'_{ij}$$

is established as a critical value criterion for yielding in three dimensions, corresponding also to an invariant distortional strain energy criterion for an isotropic material, as pointed out by Hencky. On a von Mises–Hencky basis, the flow stress of a material is independent of hydrostatic pressure, as reported experimentally for metals by Bridgman [20]. Hill [21] has laid out a mathematical description of J_2 and related plasticity considerations. Drucker [22] approached the problem from a thermodynamics viewpoint and proposed on a conservation of energy basis that the net work done by external forces during an entire cycle of load application and removal should have to be either positive or zero, never negative. This led to the Drucker–Prager postulate for plastic deformation, also described as "plastic potential theory." A consequence of the postulate is that strain (and strain rate) increments are perpendicular to the yield surface at points of stress intersections:

$$d\epsilon_{ij}^{(p)} = \lambda \frac{\partial f}{\partial \sigma_{ij}}$$

This is shown in Figure 1.4*a* for a simple two-dimensional case. The postulate is important in three-dimensional computational codes in which deformation moves back and forth across the plastic boundary. The corresponding three-dimensional yield surface is shown in Figure 1.4*b*. A corollary of the Drucker–Prager postulate is that the yield surface has to be convex.

1.3 COMMON LANGUAGE

An important bridge between dislocation mechanics and materials science was established by crystal deformation studies pioneered in the 1950s at Stuttgart and Cambridge. Hirsch's electron microscopy investigations and Seeger's dislocation model analyses of deformation tests, summarized by Seeger [23], pro-

TABLE 1.1 Mechanics–Materials Terminology

Materials	Mechanics
	Stress
True stress	Cauchy stress
Nominal stress	Kirchhoff–Piola stress
	Strain
True strain	Almansi strain
Nominal strain	Stretch
Cauchy strain	Green strain
	Other
Large deformation	Finite deformation
Small deformation	Infinitesimal deformation
Tensile test	One-dimensional straining
von Mises yield	J_2 flow
External loads	Tractions
Bauschinger effect	Kinematic hardening
Thermally activated flow	Viscoplasticity

duced complementary results. Critical TEM observations were in agreement with dislocation model predictions. Basic parameters of dislocation Burgers vectors and dislocation densities were identified and measured. Such focus on dislocation defects produced a natural connection between the language of microstructural characterization and the mechanics of dislocation strain fields, their interactions and motions. Now, there is concern for the common language requirements of the materials and mechanics community. The intersection of knowledge between the materials and mechanics communities needs to be broadened. Table 1.1 shows example comparative terms from the disciplines of mechanics and materials science.

1.4 THE CHEMISTRY–PHYSICS–MATERIALS CONNECTION

The concept of thermally activated crystal dislocation motion was involved intimately in the proposed basis for explaining the temperature and strain rate dependence of crystal plasticity, by Orowan [24] and Polanyi [25], as compared with the stronger mechanics-based Taylor [26] explanation of single-crystal stress–strain behavior. Such considerations of thermal activation have been put into practice by the materials community in the modern form of temperature and strain rate effects leading to the experimental evaluation of activation enthalpies and entropies and, also, use of Zener–Hollomon, Larson–Miller, or Sherby–Dorn graphics in analysis and prediction of material performances and

lifetimes. The fundamental concept of thermally activated defect mechanisms is applicable to both low-temperature deformation [e.g., the yield stress of body-centered cubic (BCC) metals] and high-temperature plasticity (e.g., creep deformation properties), as displayed in the deformation maps of Frost and Ashby [27] that are put to practical use. The monograph by Kocks et al. [28] provides a useful description of different rate-dependent mechanisms.

Starting from the distribution of states in a microcanonical ensemble, a generalized rate constant equation is obtained that is typically of the same form associated with the thermodynamically based van't Hoff reaction isotherm:

$$k = (\nu) \exp\left(-\frac{\Delta G}{kT}\right)$$

where ν is a frequency factor and ΔG is the Gibbs free energy of activation. The modern use of the equation for mechanisms and processes is widespread:

- Chemical reactions [29]
- Dislocation motion [30, 31]
- Phase transformation theory [32]
- Computational plasticity [33]
- Diffusional processes [34]

It may appear to give the impression that data are plotted according to a simple Arrhenius fit, but this is not so. The analysis has a sound foundation in statistical mechanics. Figure 1.5 gives a current computational application obtained with the computer EPIC program. The complete deformation shape of an Armco iron cylinder impact (Taylor) test is shown to have resulted from temperature and strain-rate-dependent viscoplastic flow by slip that followed after an initial amount of athermal flow involving deformation twinning. Additional thermal activation considerations enter into the presentations of Chapters 7, 10, 13, and 14, by Argon, Armstrong, Weertman, and Meyers, respectively.

It has been correctly stated that

Mechanics + materials = design

After all, the aim of the materials scientist is to use an understanding of mechanics to improve the performance of available materials and to design better material structures. These are not an aim in themselves, but are made to serve in some application. These sciences are application-driven. A good example of desired mechanics-materials linkage, although approached from the materials side, are the books by Gibson and Ashby [35] on cellular materials, Ashby's [36] book on material selection in mechanical design, and Frost and Ashby's [27] book on deformation mechanism maps. Although they present few new

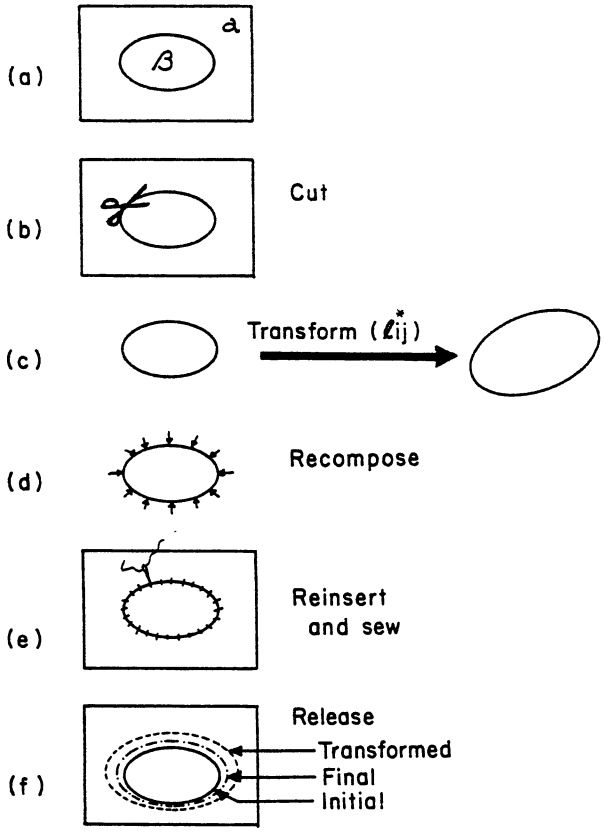


Figure 1.5 Cylinder impact (Taylor) test result (dotted shape) in comparison with EPIC-model calculation (solid shape) incorporating independently determined constitutive equations for thermally activated deformation by slip after athermal deformation twinning occurred. (From R. W. Armstrong and F. J. Zerilli, *J. Phys. Coll.* **49** (1988), C3–529.)

concepts and information in themselves, they succeed in linking critically and very productively basic concepts for the higher aim of an actual understanding. Sophisticated description is replaced by pedagogical display. The ingenious graphical "maps" have inspired a number of new lines of research.

1.5 MECHANICS OF MATERIALS

Some of the most difficult problems to deal with in mechanics involve singularities where either stress or strain (or both) approach infinite values. In order to overcome such generally unrealistic conditions, appropriate mathematical methods of solution, such as the Gauss divergence theorem, are employed to cir-

cumvent the singularity. The Gauss theorem is necessary for formulation of the Maxwell equations for electromagnetic theory. Difficulty with establishing the energy emanating from a point source is handled by moving to a certain distance, defining a surface around the singular point source, and estimating the flow of energy through the surface. The Gauss divergence theorem is a basic ingredient for the construction of the energy-momentum tensor (also introduced by Maxwell). Gauss' divergence theorem has the following form:

$$\int_V \frac{\partial \sigma_{jk}}{\partial x_i} = \int_S n_i \sigma_{jk} dS$$

where V and S are the volume and convex surface, respectively, and n_i is the unit normal vector to the surface.

Eshelby [37] first introduced the energy-momentum tensor to the mechanics community. Eshelby utilized the (Maxwell) energy-momentum tensor to define a force on the interface between an inhomogeneity and the matrix. Such forces on interfaces soon became ingredients for theories of instability and coarsening of precipitates. Application of the energy-momentum tensor to lattice defects (but not explicitly to cracks), was followed by the later J-integral theory (Cherepanov [38] and Rice [39]) and, because of incorporation into ASME codes (Begley and Landes [40]), has become accepted practice in fracture mechanics applications. Another application by Eshelby [41] dealt with the hardening mechanism associated with precipitates and inclusions. Using a sequential cutting, imposed deformation, and insertion procedure for an elliptical inclusion, as indicated in Figure 1.6, the problem of determining the entire state of stress and strain was shown to be greatly simplified. The stresses inside the inclusion are constant and outside of the inclusion are given by a so-called Eshelby tensor [Mura [42]]. This formalism has also been applied to a variety of materials problems, ranging from precipitates, martensitic transformations, mechanical twinning, and composites. The schematic procedure (for the "gedanken experiment") is as follows: the region B (Figure 1.6*a*), that corresponds to an inclusion, is removed (Fig. 1.6*b*) from the material and transformed, by dilatation and shear (Fig. 1.6*c*), and then is pushed back to its original shape by external forces (Fig. 1.6*d*), and reinserted into the hole. Imaginary surgeons dutifully reattach the inclusion to the surrounding material (Fig. 1.6*e*). On release of the surface traction, the inclusion relaxes to an intermediate shape. The same basic idea has been applied to more complicated situations (Asaro and Barnett [43]). With this approach, taken together with Khachaturyan's work [16], the theory of precipitation is one of the best understood subjects in mechanics and materials science. The understanding of inclusions and inhomogeneity problems has opened the way to various very useful applications, including the design of composites and structural ceramics, which by now have become important industries.

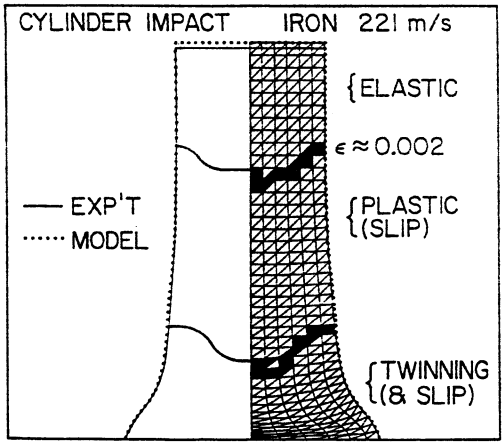


Figure 1.6 Schematic representation of operations involved in Eshelby transformation on an ellipsoidal inclusion.

1.6 OTHER MILESTONES

Such interesting results in the elastic description of heterogeneous inclusions suggested that even more relevant effects could be made use of as far as their plasticity is concerned. Deformation twinning in BCC and face-centered cubic (FCC) metals, when modeled on an Eshelby inclusion basis, necessarily involves inclusion shear strains of 0.7071, that must produce additional plasticity in the encompassing matrix material. The basic idea of engineered composite materials is to design advantageously shared loads or displacements within a material between matrix and inclusions, so as to fully utilize the positive attributes of both materials. This field already connects with engineering practice; composites are being manufactured for items from military transportation and medical uses to recreational applications. Current understanding of composite behavior has been very much refined, but most of the basic ideas can be found in Kelly's [44] book *Strong Solids*. Here again, the key to this success story occurs in the fact that a combination of mechanics and materials science approaches have led in a number of pioneering examples to the obtainment of high performance materials.

In another example, the field of structural ceramics has profited immensely from Eshelby's theory of heterogeneous inclusion behaviors. At the intersection of mechanics and materials, seminal contributions of Heuer et al. [45] and Evans and Langdon [46] come to mind. Similar developments appear to be occurring in the subject areas of biomaterials and bioengineering. Cellular solids [Gibson and Ashby [35]], including artificial materials akin to biological ones, are put to use for a wide variety of nonbiological applications. At the same time, use of high-technology materials for biological purposes (heart valves, artificial skin and bones, prostheses in general) is rapidly increasing [47]. In these endeavors,

the mechanics of materials is being utilized within new environments. The next step is to copy (or mimic) biological systems: this is the field of biomimetics [48].

1.7 CURRENT PRACTICE

Mechanics and materials science are moving together in several other modern instances, such as for electronic devices in very large-scale integration (VLSI) designs. In the military domain, the design and optimization of penetrators and armor require a constant interplay between mechanics and materials. Solid free-forming and molecular-beam epitaxy (MBE), as one method of nanoscale layer deposition, are other areas where this cooperation of joint tools and methods are about to expand. The current availability of a wide range of materials, from metals to ceramics to organics, concrete and biological materials, will necessarily require the use of appropriately realistic constitutive laws. These will undoubtedly be more sophisticated and compiicated than those in use today and contribute to further advances in tailored processing and design of materials for special mechanics applications.

The research effort developed from the 1950s to establish a microscopic defect model for macroscopic plasticity has been only partly successful. The central agenda, to understand the three stages of work hardening of single crystals in order to more fully understand and describe polycrystalline deformation and, thence, to handle problems of large-scale deformation and fracturing, remains to be completed. Enormous advances were made in dislocation theory in that the properties and behavior of individual dislocations are now well understood, but their collective behavior has been addressed with only partial success. Cottrell [49], while making seminal contributions to the effort, prophetically stated that "it was one of the first problems to be tackled and one of the last ones to be solved." Taylor's [50] description of a square root of strain dependence for the polycrystal plastic flow stress continues to be a widely accepted approximation. The Hall–Petch linear relation for the dependence of the yield stress and fracture stress of steel on the reciprocal square root of average grain diameter, although generalized to describe the complete stress–strain behaviors of most metals and alloys [51], is not uniquely attributed to the original dislocation pileups and needs to be more fully rooted in mechanics analyses.

The incorporation of statistical mechanics considerations for very flexible dislocation line structures is needed for both strain and grain size dependencies. Impressive computer simulations by the French school have addressed this problem, but thus far have necessarily needed to restrict the dislocation microstructures to an assemblage of relatively stiff, segmented line elements. The complete simulation of a microstructure during large scale deformation is known to require the full capacity of modern computers, though progress is being made as described here in Chapter 8 by Anand. The difficulty in obtain-

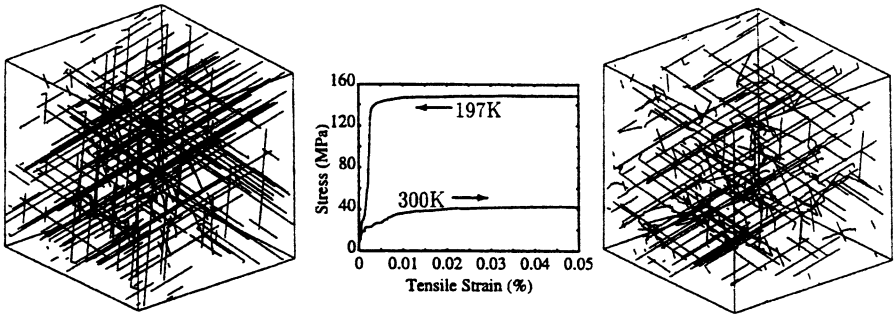


Figure 1.7 Dislocation dynamics simulation of plastic deformation in BCC single crystals (Ta). The stress–strain curves (center) are obtained at 197 K (at left) and 300 K (at right). The initial dislocation density is 10^{11} m^{-2}. Notice that the dislocation microstructures are different at the two temperatures. At low temperature (197 K), it consists mainly of elongated screw dislocations. At high temperature (300 K), the proportion of short edge dislocations increases. This difference in dislocation microstructure originates from the difference in the relative dislocation mobilities at low and high temperatures. (From M. Tang, L. P. Kubin, G. R. Canova, *Acta Materialia*, 46 (1998) 3221).

ing "the complete story" of defect mechanics in linkage from the nanoscale to the mesoscale and then to the macroscale must involve spatial resolution over the nine orders of magnitude mentioned earlier in this presentation [52]. Valid constitutive equations are needed for the total range in scale. This remains a challenging problem that probably will be solved by combined use of computational and, at least, semi-analytical techniques. Figure 1.7 shows a dislocation dynamics simulation of tantalum at two different temperatures: 197 and 300 K. The effect of temperature on the evolution of dislocation organization is clear. It is expected that calculations such as these by Tang et al. [53], will lead to a much better prediction of the mechanical response of materials. In the meantime, we look forward with our mechanics and materials colleagues to continued progress in understanding the properties of materials in terms of their consolidating forces at the finest scale and, with this knowledge, more fully utilizing the total range of accessible material properties in advanced engineering applications.

REFERENCES

1. I. Todhunter and K. Pearson, *A History of the Theory of Elasticity and of the Strength of Materials*, Cambridge Univ. Press, 1886.
2. A. E. H. Love, *A Treatise on the Mathematical Theory of Elasticity* (1927), 4th ed., Cambridge Univ. Press, 1959.
3. C. A. Truesdell, *Essays in the History of Mechanics*, Springer, New York, 1968.

4. S. Timoshenko, *History of Strength of Materials*, Dover, New York, 1983.
5. J. R. Rice, "Mechanics of Solids," *Encyclopaedia Britannica, Macropaedia*, Vol. 23, Encyclopaedia Britannica, Inc., Chicago, 1993, p. 734.
6. F. Seitz, *Physics of Metals*, McGraw-Hill, New York, 1940.

6a. C. S. Barnett, *Structure of Metals*, McGraw-Hill, New York, 1943.

7. E. Orowan, *Instn. Eng. Shipb. Scotland* **89** (1945/46), 165.
8. P. B. Hirsch, R. W. Horne, and M. J. Whelan, *Phil. Mag.* **1** (1956) 677.
9. W. Bollmann, *Phys. Rev.* **103** (1956) 1588.
10. H. Mughrabi, in *Constitutive Equations in Plasticity*, A. S. Argon, ed., Cambridge, MA, MIT Press, 1975, pp. 199–243.
11. X. J. Zhang, R. W. Armstrong, and G. R. Irwin, *Met. Trans.* **20A** (1989), 2863–2864.
12. A. Guinier, *Nature* **142** (1938), 569.
13. G. D. Preston, *Nature* **142** (1938), 570.
14. O. Blaschko, R. Glas, G. Krexner, and P. Weinzierl, *Acta met. mat.* **42** (1994) 43–50.
15. V. Groeger, P. Fratzl, W. Pahl, O. Paris, G. Bischof, and G. Krexner, *Acta met. mater.* **43** (1995) 1305–1311.
16. A. G. Khachaturyan, *Theory of Structural Phase Transformations in Solids*, Wiley, New York, 1983.
17. R. Glas, M. Jouiad, P. Caron, N. Clement, H. O. K. Kirchner, *Acta Mat.* **44** (1996), 4917–4926.
18. E. Ruska, *The Early Development of Electron Lenses and Electron Microscopy*, S. Hirzel Verlag, Stuttgart, 1980.
19. A. Cerezo, T. J. Godfrey, C. R. M. Grovenor, M. G. Hetherington, J. M. Hyde, J. A. Liddle, R. A. D. Mackenzie, and G. D. W. Smith, *EMSA Bull.* **20**[2], (1990) 77–83.
20. P. W. Bridgman, *Proc. Am. Acad. Art. Sci.* **58** (1923) 163–242.
21. R. Hill, *The Mathematical Theory of Plasticity*, Clarendon Press, Oxford, 1950.
22. D. C. Drucker, *Proc. 1st Natl. Congress Appl. Mech.*, Chicago, 1951, pp. 487–491.
23. A. Seeger, *Kristallplastizitat, Handbuch der Physik* VII/2, *Crystal Physics* II, S. Flugge, ed., Springer, Berlin, 1958, p. 541.
24. E. Orowan, *Zeits, Phys.* **89,** 1934, 605,634.
25. M. Polanyi, *Zeits. Phys.* **89,** 1934, 660.
26. G. I. Taylor, *Proc. Roy. Soc. Lond.* **A145,** 1934, 362.
27. H. J. Frost and M. F. Ashby, *Deformation-Mechanism Maps*, Oxford Univ. Press, Oxford, 1988.
28. U. F. Kocks, A. S. Argon, and M. F. Ashby, *Progress in Materials Science*, Vol. 19, B. Chalmers, J. W. Christian, and T. B. Massalski, eds., Oxford Univ. Press, Oxford, 1975.
29. H. Eyring, *Modern Chemical Kinetics*, Reinhold, New York, 1963.
30. G. Schoeck, in *Dislocations in Solids*, Vol. 3, F. R. N. Nabarro, ed., North-Holland, Amsterdam, 1976.
31. A. S. Krausz and H. Eyring, *Deformation Kinetics*, Wiley, New York, 1975.

32. J. W. Christian, *The Theory of Transformations in Metals and Alloys*, Pergamon Press, Oxford, 1981.
33. F. J. Zerilli and R. W. Armstrong, *J. Appl. Phys.* **61** (1987), 1816.
34. J.-M. Penisson and J. Philibert, *Atom Movements*, Editions de Physique, Les Ulis, 1991.
35. L. J. Gibson and M. F. Ashby, *Cellular Solids*, Pergamon Press, Oxford, 1988.
36. M. F. Ashby, *Materials Selection in Mechanical Design*, Pergamon Press, Oxford, 1992.
37. J. D. Eshelby, *Phil. Trans. Roy. Soc. Lond.* **A244,** 1952, 87–112.
38. G. P. Cherepanov, *Appl. Math Mech.* **31** (1967), 503.
39. J. R. Rice, *J. Appl. Mech.* **35,** 1968, 379–386.
40. J. A. Begley and J. D. Landes, *ASTM STP514*, ASTM, Philadelphia, 1972, p. 1.
41. J. D. Eshelby, *Proc. Roy. Soc. Lond.* **A252** (1959), 561.
42. T. Mura, *Micromechanics of Defects in Solids*, 2nd. ed., Nijhoff, Lancaster, 1987.
43. R. J. Asaro and D. M. Barnett, *J. Mech. Phys. Sol.* **23** (1975), 77–83.
44. A. Kelly, *Strong Solids*, 3rd ed., Clarendon Press, Oxford, 1986.
45. A. H. Heuer, F. F. Lange, M. V. Suarh, and A. G. Evans, *J. Am. Cer. Soc.* **69** (1986).
46. A. G. Evans and T. G. Langdon, "Structural Ceramics," *Progr. Mat. Sci.* **21** (1976), 171.
47. Y. C. Fung, *Biomechanics: Mechanical Properties of Living Tissues*, 2nd ed., Springer, New York, 1995.
48. J. V. Vincent, *Structural Biomaterials*, Princeton Univ. Press, Princeton, NJ, 1991.
49. A. H. Cottrell, *The Mechanical Properties of Matter*, Wiley, New York, 1964.
50. G. I. Taylor, *J. Inst. Metals* **62** (1938), 307.
51. R. W. Armstrong, I. Codd, R. M. Douthwaite, and N. J. Petch, *Philos. Mag.* **7** (1962), 45–53.
52. H. O. Kirchner, L. P. Kubin, and V. Pontikis, eds., *Computer Simulation in Materials Science: Nano/Meso/Macroscopic Space and Time Scales*, NATO ASI Series E, Applied Sciences, Vol. 308. Kluwer Academic Publishers, Boston, 1996.
53. M. Tang, L. P. Kubin, and G. R. Canova. *Acta Mat. 46*, (1988) 3221.

Ed: 46(1988)5?