2. Computational design of materials with extreme mechanical properties

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2.1 Ab initio elasticity of single-crystal solids

The most general linear relationship which connects stress to strain is provided by the generalized version of the well-known Hooke's law

$$\sigma_{mn} = C_{mnij} \varepsilon_{ij}$$

in which σ_{mn} denotes the stress tensor, ε_{ij} the strain tensor and the elements of the

fourth-order tensor C_{mnij} are the so-called elastic constants. The knowledge of these data may

enable prediction of mechanical behavior in many different situations. Whereas σ_{mn} and ε_{ij}

are symmetric and have therefore only 6 independent elements, the number of C_{mnii} is

reduced by symmetry arguments to a total of 21. The elastic energy density u, which is defined as the total energy per volume, is obtained from the stress tensor (force per unit area) by integration of Hooke's law

$$e_{tot} = E_{tot} / V = \frac{1}{2} C_{mnij} \varepsilon_{mn} \varepsilon_{ij} = \frac{1}{2} C_{\alpha\beta} \varepsilon_{\alpha} \varepsilon_{\beta}$$

The strain tensor has been considered as a tensor of order two of the form

$$\varepsilon = \begin{bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{bmatrix}.$$

Taking into account additional symmetry arguments imposed by the crystal lattice, the number of elastic constants further decreases. In particular, for a cubic lattice only three independent

elastic constants,

$$C_{\alpha\beta}(cubic) = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix}$$

remain, whereas for a tetragonal lattice C_{mnij} contains six elastic constants

$$C_{\alpha\beta}(tetragonal) = \begin{bmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{66} \end{bmatrix}.$$

There are two ways of computing single crystal elastic constants from *ab initio* methods: the *energy-strain* approach and the *stress-strain* approach. The *energy-strain* approach is based on the computed total energies of properly strained crystal. For each strain type, several magnitudes of strains are applied and the corresponding total energies are computed with an *ab initio* approach. The stiffness is then derived from the curvature of the *energy-strain* relation by means of a least-squares fit. Some of the imposed strains may be related to a single elastic constant while others are described by a linear combination of elastic constants, from which the elastic tensor is evaluated. The number of necessary distortions is given by the number of independent elastic constants.

As an example, the deformations used for the calculation of the elastic constants in a cubic crystal are discussed. Note that the linear elastic *energy-strain* relation is valid for any crystal symmetry, and by that it is possible to evaluate elastic constants of any crystalline material. The elastic energy density for a cubic crystal can be expressed as

$$e_{tot} = \frac{1}{2}c_{11}(\varepsilon_{11}^2 + \varepsilon_{22}^2 + \varepsilon_{33}^2) + \frac{1}{2}c_{44}(\varepsilon_{23}^2 + \varepsilon_{31}^2 + \varepsilon_{12}^2) + c_{12}(\varepsilon_{11}\varepsilon_{22} + \varepsilon_{33}\varepsilon_{22} + \varepsilon_{11}\varepsilon_{33}).$$

Note that a cubic crystal shown below



has a = b = c, and $\alpha = \beta = \gamma = 90^{\circ}$. A tetragonal distortion can be generated by distorting

the cubic crystal along the c-axis. The resulting tetragonal crystal lattice is shown as



has a crystal structure of $a = b \neq c$, and $\alpha = \beta = \gamma = 90^{\circ}$. Under the tetragonal distortion, the shear displacements will be zero and the diagonal components of the strain tensor can be expressed as

$$\varepsilon_1 = \varepsilon_2 = da/a, \varepsilon_3 = dc/c, \varepsilon_4 = \varepsilon_5 = \varepsilon_6 = 0$$

The elastic energy density $e_{tot} = \frac{1}{2} C_{\alpha\beta} \varepsilon_{\alpha} \varepsilon_{\beta}$ becomes

$$\begin{split} e_{tot} &= (c_{11} + c_{12})\varepsilon_{11}^2 + 2c_{12}\varepsilon_{11}\varepsilon_{33} + \frac{c_{11}}{2}\varepsilon_{33}^2 \\ &= \frac{c_{11} + 2c_{12}}{6}(\frac{dV}{V})^2 + \frac{2(c_{11} - c_{12})}{6} \bigg(\frac{d(c/a)}{c/a}\bigg)^2 \end{split}$$

Therefore, we can determine c_{11} and c_{12} from the energy-strain relationship using different magnitudes of tetragonal distortion.

A trigonal lattice shown as



can also be produced by distorting a cubic crystal along its [111] direction to yield a crystal structure of a = b = c, and $\alpha = \beta = \gamma \neq 90^{\circ}$. The total energy density from this triangle

deformation can be deduced in terms of c/a and V as $e_{tot} = \frac{c_{11} + 2c_{12}}{6} \left(\frac{dV}{V}\right)^2 + \frac{2c_{44}}{3} \left(\frac{d(c/a)}{c/a}\right)^2$.

Thus, the shear constant $G=c_{44}$ can be determined from the energy-strain relationship with different magnitudes of triangle deformation. Here we choose the trigonal and tetragonal distortions, because they preserve as much symmetry as possible and, thus, reduce

computational costs and guarantee a high precision. The choice of distortions is analogous for crystals with other symmetries.

To determine the bulk modulus B of a crystal, we assume the crystal is subjected to hydrostatic isotropic compression. By calculating the curvature at the equilibrium volume V_0

the bulk modulus *B* can be directly derived as $B = \frac{1}{3}(c_{11} + 2c_{12}) = V \frac{\partial^2 E}{\partial V^2}\Big|_{V_0}$.

The *stress-strain* approach directly calculates the stress tensor. Once the stress tensor components are obtained by an *ab initio* method, the elastic constants matrix can be directly derived from the generalized Hooke's law. For instance, assuming again cubic symmetry, the elastic constants can be expressed in terms of the stress tensor by

$$\begin{split} c_{44} &= \frac{1}{2} \frac{\partial \sigma_{12}}{\partial \varepsilon_{12}} \\ \frac{1}{2} (c_{11} - c_{12}) = -\frac{1}{2} \frac{\partial \sigma_{33}}{\partial \varepsilon_{33}} \\ B &= \frac{1}{3} (c_{11} + 2c_{12}) = \frac{\partial \sigma_{11}}{\partial \varepsilon_{11}} \end{split}$$

Whereas within the *energy-strain* approach several magnitudes of strain have to be evaluated in order to obtain the elastic constant from an analytic fit to the total energy data, within the stress-strain approach just one evaluation is sufficient to obtain the same information.

By macroscopic averaging, elastic moduli of polycrystalline materials can be derived. There are several averaging procedures available to derive the elastic moduli of a quasi-isotropic polycrystalline material from its single crystal elastic constants. The averaging encumbers all possible orientations of the crystal, and there is a well-defined lower and upper limit for the elastic moduli. Based on the averaging procedures, the *ab initio* treatment for single crystals can be extended to polycrystalline samples.

Case study: ab initio calculation of elastic properties of BN.

2.2 Superhard materials

For details, see lecture note 6.

2.3 Dislocation Defects in Crystal

Volterras reported that an arbitrary deformation of an arbitrary body can be deduced by repeating and combining two independent cuts and shifts. A real dislocation produces exactly the strain field generated by the cut and shift procedure.

The elastic distortion around a straight screw dislocation (left) of infinite length can be represented in terms of a cylinder of elastic material deformed as illustrated in the right figure below:



Because in the core region of a dislocation the strain is very large, where atoms are displaced by about a lattice constant, linear elasticity theory thus is not a valid approximation in the core region. We then have to consider the core region separately and add it to the solutions from linear elasticity theory.

The elastic field in the dislocated cylinder can be found by noting that there are no displacements in the x and y directions, i.e., $u_x = 0$, $u_y = 0$. In the z-direction, the displacement varies smoothly from 0 to b as the angle θ goes from 0 to 2π . This can be expressed as

$$u_z = \frac{b}{2\pi} \cdot \theta = \frac{b}{2\pi} \tan^{-1}(y/x).$$

Using the equations for the strain we obtain the strain field of a screw dislocation:

$$\begin{split} \varepsilon_{xx} &= \frac{\partial u_x}{\partial x} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon_{xy} = \varepsilon_{yx} = 0\\ \varepsilon_{xz} &= \frac{1}{2} \left[\frac{\partial u_z}{\partial x} + \frac{\partial u_x}{\partial z} \right] = -\frac{b}{4\pi} \cdot \frac{y}{x^2 + y^2} = -\frac{b}{4\pi} \cdot \frac{\sin \theta}{r} \\ \varepsilon_{yz} &= \frac{1}{2} \left[\frac{\partial u_z}{\partial y} + \frac{\partial u_y}{\partial z} \right] = \frac{b}{4\pi} \cdot \frac{x}{x^2 + y^2} = \frac{b}{4\pi} \cdot \frac{\cos \theta}{r} \end{split}$$

The corresponding stress field is also easily obtained from the generalized Hooke's law

$$\sigma_{\alpha} = C_{\alpha\beta}\varepsilon_{\beta} = C_{\alpha\beta}(cubic) \cdot \varepsilon_{\beta} = \begin{bmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 0 \\ \frac{b}{2\pi} \cdot \frac{\cos\theta}{r} \\ -\frac{b}{2\pi} \cdot \frac{\sin\theta}{r} \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{C_{44}b}{2\pi} \cdot \frac{\cos\theta}{r} \\ -\frac{C_{44}b}{2\pi} \cdot \frac{\sin\theta}{r} \\ 0 \end{bmatrix}$$

with $C_{44} = G$.

The stress can be expressed in cylindrical coordinates as

$$\sigma_{rz} = \sigma_{xz} \cos \theta + \sigma_{yz} \sin \theta = 0, \\ \sigma_{\theta z} = -\sigma_{xz} \sin \theta + \sigma_{yz} \cos \theta = \frac{Gb}{2\pi r}.$$

The stress field exhibits complete radial symmetry and the cut thus can be made on any radial plane θ = constant. However, a serious problem occurs: The stresses and strains are proportional to 1/r and therefore diverge to infinity as $r \rightarrow 0$ as shown in the following schematic picture.



Therefore, the cylinder must be hollow to avoid *r*-values that are too small, *i.e.*, smaller than the core radius r_0 .

The stress field of an edge dislocation can also be represented in an isotropic cylinder. We replace the edge dislocation by the appropriate cut in a cylinder. The displacement and strains in the z-direction are zero and the deformation is basically a "plane strain".



The stress field of the edge dislocation can be depicted as

$$\sigma_{xx} = -D \cdot y \frac{3x^2 + y^2}{(x^2 + y^2)^2}, \quad \sigma_{yy} = D \cdot y \frac{x^2 - y^2}{(x^2 + y^2)^2} \quad \sigma_{xy} = \sigma_{yx} = D \cdot x \frac{x^2 - y^2}{(x^2 + y^2)^2},$$

With $D = Gb/[2\pi(1-\nu)]$, the stress field has both dilational and shear components. The

largest normal stress is σ_{xx} which acts parallel to the Burgers vector. Since the slip plane can be defined as y = 0, the maximum compressive stress (σ_{xx} is negative) acts immediately above the slip plane and the maximum tensile stress (σ_{xx} is positive) acts immediately below the slip plane.

The energy of a dislocation comes from the elastic part that is contained in the elastically strained bonds outside the radius r_0 and from the energy stored in the core, which is of course energy sitting in the distorted bonds, too, but is not amenable to elasticity theory. The total energy per unit length E_{ul} is the sum of the energy contained in the elastic field, E_{el} , and the energy in the core, E_{core} . The strain energy for a volume element will give the total elastic energy E_{el} of the dislocation. The integration is easily done for the screw dislocation; in what follows the equations are always normalized to a unit of length

$$\begin{split} E_{el}(screw) &= \int dE_{el}(screw) = \int_{r_0}^R \pi r (\sigma_{\theta z} \varepsilon_{\theta z} + \sigma_{z\theta} \varepsilon_{z\theta}) dr = \int_{r_0}^R 4\pi r G \cdot (\varepsilon_{\theta z})^2 dr \\ &= \frac{G \ b^2}{4\pi} \ln \frac{R}{r_o} \\ E(edge) &= \frac{G \ b^2}{4\pi (1-\nu)} \ln \frac{R}{r_o} \end{split}$$

The integration runs from r_0 (the core radius of the dislocation) to *R*, which is some as yet undetermined external radius of the elastic cylinder containing the dislocation. The line energy of an edge dislocation is always larger than that of a screw dislocation since (1 - v) < 1. With $v \approx 1/3$, we have $E(\text{screw}) \approx 0.66 \cdot E(\text{edge})$. Taking an extremely small value for r_0 to be 0.1 nm, a realistic range for *R* as 100 µm-10 nm, we obtain $\ln (R/r_0) = 13.8 - 4.6$. We now deduce an approximation for the line energy that is sufficiently good for most purposes. The best simple value for the core energy

is $E_{core} = G b^2 / 2\pi$. Thus, in a very general way we can write $E_{tot} \simeq G b^2$ for the total elastic energy of a dislocation.

2.4 *ab initio* Modeling of Brittle and Ductile Behavior of Solids

In advanced electrical and mechanical devices, as the size of critical components shrinks, and the demands for high performance and reliability increase, a detailed understanding of the microscopic processes responsible for ductile or brittle behavior becomes increasingly important. In brittle solids, the imposition of external stress results in the extension of pre-existing cracks: the stress concentration at the crack tip, leads to bond-breaking and cleavage. In contrast to this, in a ductile substance the large stress at the crack tip is absorbed by generation and motion of dislocations which blunts the crack; the net effect is plastic deformation of the material but no breaking.

What would it take to actually simulate at the microscopic level the processes responsible for brittle or ductile behavior? We would need to include in the simulation a large enough number of atoms to capture the different types of defects (cracks, dislocations, surfaces, grain boundaries, point defects) and their response to external loading, at finite temperature. This is impossible with current computational capabilities. In the classical molecular dynamic simulation, the complex interaction between atoms is reduced to a few-body interatomic potential which depends on atomic distances and the angles between such distances. It is not clear to what extent this simplified description can capture realistically the atomistic processes responsible for bond breaking and cleavage (in the case of a brittle solid) or dislocation nucleation and motion (in the case of a ductile solid). Alternatively, one can use sophisticated quantum mechanical methods for describing the properties of solids at the atomic level. Direct application of these methods yields an accurate description of the electronic and atomic structure of bulk crystals, their simple surfaces and interfaces, of small clusters of atoms, etc. Properties that represent small perturbations from the equilibrium crystal structure of the solid, such as the phonon spectrum, elastic moduli, optical, dielectric and magnetic constants, can also be obtained with reasonable accuracy. At present, these calculations are limited to systems of order a few hundred atoms. It is clear from the above discussion that successful modeling of physical phenomena which involve atomistic processes and their implications for macroscopic behavior, must rely on a combination of methodologies. A simpler approach to partially fulfill this goal is to use results from phenomenological macroscopic theories coupled with first-principles quantum mechanical calculations to determine the values of any physical parameters that enter in the phenomenological description.

2.4.1 Macroscopic Theory of Brittle versus Ductile Behavior of a Solid

The concept of the generalized stacking fault energy surface (i.e., γ -surface), originally introduced by Vitek, is central to many macroscopic theories of plastic deformation. Consider a crystal cut into two halves parallel to the (*hkl*) crystallographic plane and suppose that one half is displaced relative to the other by a vector v. The plane (*hkl*) is called the fault plane and v=0 corresponds to the ideal crystal, the minimum energy configuration. The change in energy per unit area of the crystal as a function of v, which is varied on the (*hkl*) plane to scan a unit cell, is called the γ -surface. The γ -surface is a fundamental material property which can be obtained from atomistic calculations.

A useful description of dislocation motion was proposed by Peierls and Nabarro. Peierls-Nabarro model represents the crystal dislocation as a continuous, planar distribution of infinitesimal disregistry of atomic planes on either side of a fault plane. The density of this

disregistry $\rho(x)$ is given in terms of the displacement field $\vec{u}(x)$ as $\rho(x) = \left| d\vec{u}(x) / dx \right|$. The

balance between the forces among the infinitesimal segments of the dislocations and the elastic restoring force of the crystal leads to

$$K \int_{-\infty}^{+\infty} dx \, \frac{d\vec{u}(x')}{dx'} \frac{1}{|x-x'|} = -\nabla_{\vec{u}} \gamma \left[\vec{u}(x)\right]$$

with
$$\int_{-\infty}^{+\infty} dx \, \frac{d\vec{u}(x')}{dx'} = \vec{u}(\infty) - \vec{u}(-\infty) = \vec{b}$$
 (2.4.1)

Here, *K* is an elastic constant and \vec{b} is the Burgers vector of the dislocation. Eq. (2.4.1) relates the stress on the lattice at a position *x* due to the infinitesimal dislocation distribution at that point $\vec{u}(x)$ to the force exerted by the lattice due to its distortion, which is given by the gradient of the γ -surface. Consider when this distribution of lattice disregistry is moved by a distance equivalent to the lattice periodicity and compute the change in energy as a function of *x*. This energy cost can be related to the external stress required to move the dislocation. This energy is referred to as the Peierls energy $W_P(x)$ and its maximum gradient is the Peierls stress for translation of rigid dislocations at zero temperature. In the limit of narrow dislocations, the Peierls stress is given directly by the maximum gradient of the γ -surface along an extremal

path over which the displacement vector \mathbf{v} varies continuously from 0 to \vec{b} .

2.4.2 Ductility versus brittleness

The competing processes which lead to brittle or ductile behavior are the extension of the

crack by creation of fresh surfaces (brittle response) or the generation of dislocations that exert a back stress which reduces the stresses by blunting the crack tip (ductile response). Most solids can undergo a transition between brittle and ductile response, which can be very sharp as a function of temperature.

In brittle failure, the energy required for an incremental advance of the crack front is given by the Griffith criterion: $G = 2\gamma_s$, where G is the energy release rate (the mechanical

energy released per unit area swept by the crack front) and γ_s is the surface energy (the energy needed to create a unit area of fresh surface).

Kelly and coworkers were the first to rationalize the distinction between brittle and ductile behavior by postulating that a material would be ductile if the crack tip stress exceeded the theoretical shear stress before the theoretical tensile stress was reached. A direct linkage to the ductile-to-brittle transition (DBT) was made later by Rice and Thomson (the RT model), who proposed that the onset of ductile behavior occurred when spontaneous emission of dislocations at the crack tip became feasible. In the RT model, dislocations which move more

than a critical distance a_c from the crack tip are repelled by the crack and are hence considered

to be nucleated. If a_c is smaller than the dislocation core radius a_0 , the material is considered to be ductile at all temperatures.

In a modern variant of the RT model, Rice introduced the unstable stacking fault energy γ_{us} (which shall also scale directly with Peierls stress) as the maximum energy barrier encountered along the extremal path, which connects 0 and Burgers vector on a plane (hkl). γ_{us} is a measure of the nucleation energy for a dislocation of Burgers vector on the (hkl)plane and therefore the criterion for dislocation nucleation at the crack tip (ductility) is reached when $G = \alpha \gamma_{us}$ with $\alpha \sim 1$. In an alternative model of the DBT, Hirsch and Roberts (HR) postulated that the governing mechanism is the motion of dislocations. The crack tip stresses activate internal sources, with dislocations of one sign moving into the bulk and of the opposite sign being absorbed into the crack, thus connects the DBT with dislocation mobility. This again scales with the unstable stacking fault energy γ_{us} , which can be considered to be the key parameter for dislocation related processes of ductility.

To summarize, the conditions for both brittle fracture and ductile response with the nucleation and motion of dislocations can be expressed in terms of features of the γ -surface. If

we adopt the view that *dislocation nucleation is a necessary precursor to dislocation motion*, the conditions become particularly simple, depending only on the two energies γ_s and γ_{us} .

Brittle behavior is the consequence of the condition $G=2\gamma_s$ being satisfied before the

condition of $G=\alpha\gamma_{us}$. The converse is true for ductile materials. We can then conveniently

define a disembrittlement parameter as $D = \gamma_s / \gamma_{us}$. Unfortunately, here γ_s and γ_{us} are not

provided by any analysis based on continuum arguments. They have to be established from accurate microscopic calculations. The critical value of the disembrittlement parameter D has been estimated to be between 1 (more brittle) and 10 (more ductile). One might hope that changes in D due to changes in the microscopic structure or chemical composition of a solid will correlate with changes in the solid's tendency to behave as a brittle or a ductile substance.

2.4.3 First-Principles Methods

To calculate γ_s and γ_{us} , we can use slab configurations with multiples of the unit cell along the slab direction and proportionately smaller grids of *k*-points in the corresponding direction in reciprocal space.

Surface energies γ_s can be obtained from the difference between the total energy $E_{\rm tot}$ of a

crystal cleaved across a given plane and of the bulk as $2\gamma_s = E_{tot}(\text{supercell}) - nE_{tot}(bulk)$.

Here $E_{tot}(bulk)$ is the total energy of bulk crystal per chemical unit, and $E_{tot}(supercell)$ the total energy of the given supercell, which contains *n* chemical units. The overall factor of two comes from the fact that each supercell has two surfaces.

We consider a periodic supercell containing several units of the ideal crystal cell (*e.g.*, n=6 for Si, 2 to 4 for MoSi₂) and calculate the total energy as a function of *d*, the distance between two atomic layers separated by the desired cleavage plane in the supercell. These

energies are fit to a universal energy function $\textit{e}(d) = \frac{E_{tot}(d)}{A} = e_{\infty} - 2\gamma_s(1+f)e^{-f}$,



where $f = (d - d_0) / \lambda$, e_{∞} is

the energy per unit area (A) of the cleaved crystal, d_0 is the inter-planar separation in the ideal bulk crystal and λ a fitting parameter. The unstable stacking fault energy is obtained from the total energy of a supercell containing the fault plane with the two halves of the cell displaced in the direction of the fault vector with respect to each other.



A Case Study of *ab initio* Calculation of Surface Energy γ_s on TiO₂(111)

2.5 Materials for flexible electronics (hard films on flexible substrates)

Flexible electronics is set to bring about revolutionary changes in design and conceptualization of electronics devices in the consumer and medical sectors. The wide applications of flexible electronics include paper-like electronic displays, conformable electronic textiles, rollable solar cells, adaptive RFID tags, sensor skins, and hemispheric electric eye camera.

Beyond material synthesis and circuit fabrication, the deformability of flexible electronics is a mechanics problem in the heart. Flexible electronic devices will be subject to one-time or repeated mechanical and thermal loads during manufacture, application, and maintenance. While some organic materials can recover from large strains, most inorganic electronic materials fracture at small strains, often less than about one percent. Tremendous efforts have been made to optimize configurationally design so that the hard functional components and the flexible supportive base are able to deform compatibly. Examples include polymer-supported periodic arrays of stiff islands, wrinkled electrodes or silicon thin films, as well as open mesh geometries where deformation is accommodated by in-plane rotation. The island-interconnect configuration depicted in Figure 2.5.1 uses stretchable interconnects of metal wires (orange wires) a compliant polymer substrate to link electronic components fabricated on isolated, stiff islands (green squares). The fabrication of polymer-supported islands plus interconnects is the



most straightforward and is adequate for one-time large deformation.

Failures associated with the island-interconnect structure shown in Figure 2.5.2(a) have been reported. For example, Figure 2.5.2(a) shows channel cracks in a polyimide-supported TFT made of amorphous silicon.

A silicon nitride island debonded from polyimide substrate is shown in Figure 2.5.2(b). Although metals are usually considered to be ductile, thin metal films cannot elongate infinitely. Figure 2.5.2(c) shows zigzag cracks in a copper film bonded to a polyimide substrate after an elongation of 30%. Metallic interconnects can also rupture at island edges due to island sliding, as shown in Figure 2.5.2(d). Failure of islands is detrimental to device performance because millions of transistors are supported by the islands. In addition, rupture of metallic interconnects results in loss of electrical conductivity. How to improve the deformability and reliability of the flexible electronic devices gives rise to the engineering significance of the current research.



From scientific point of view, flexible electronic systems are large structures of diverse architectures, hybrid materials, and small features. When these structures are subject to mechanical loads during manufacturing or application, two essential observations have been made: (1) A hybrid structure behaves unusually when its constituents are materials of extremely different kinds. (2) The

constituents behave differently from their bulk counterparts when features of the structure are small.

Substrate-bonded thin films behave differently compared to their free-standing counterparts. For example, free-standing metal thin films rupture at small strains by a single neck whereas polymer-supported metal sheets rupture at much larger elongations through multiple necks, accompanied by simultaneous debonding from the substrates. Ceramic thin films usually fracture by cleavage, but when an ITO film was bonded to a polymeric substrate, cracks in the film were found to grow gradually under cyclic tension. The unusual behaviors of hard inorganic thin films supported by soft polymeric substrates motivate a great interest to pursue mechanistic understandings of their deformation and failure mechanisms. Such understanding will not only expand to our knowledge of the processing-structure-property relationship, but also help us take full advantage of currently available materials in order to produce highly deformable and reliable electronic devices.