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The mechanics of electronic materials

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Abstract

The primary engineering function of electronic materials is the control of electric charge for some useful purpose, rather than any mechanical load carrying function. However, mechanical stress and its consequences are central factors in the fabrication, performance and reliability of microelectronic devices, broadly affecting one of the largest industries in the world. Here, attention is focused on the role of stress in the fabrication of semiconductor heterostructures. Particular attention is devoted to strain relaxation by dislocation formation and interaction, stress-driven surface morphology evolution, and the influence of strain on electronic transport characteristics in quantum structures relevant to the next generation of devices. © 1999 Elsevier Science Ltd. All rights reserved.

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1. Introduction

Development of the engineering science of solid mechanics is motivated largely by efforts to exploit the practical advantages of structures and machines with increased reliability and decreased cost. The principal functions of such devices are to support loads, to transmit the effects of forces over some distance, and to convert energy from one form to another.

In recent years, several research directions have emerged in the field of solid mechanics which focus on engineering systems in which load carrying capacity is not a *functional characteristic* of the system. Among these is the mechanics of electronic materials. For such systems, the primary function is control of transport of electric charge driven by applied electric fields. However, mechanical stress and its consequences are often central factors in fabrication, performance and reliability of material structures or devices for microelectronic applications. The goal here is to discuss, mostly through qualitative description of illustrative examples, a number of phenomena which arise as direct consequences of stress in electronic materials. Understanding of these phenomena is important as a guide to the manufacture of the next generation of small and efficient devices.

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Advances in the methods of deposition and characterization of crystalline films of sub-micron thickness have been dramatic over the past 25 years. To some extent, such advances have been driven by basic scientific curiosity about the properties of materials at very small size scales. From the point of view of microelectronics applications, improvements in the technology are continually pursued; for example, improvements can be sought through increases in spatial density of individual devices on a chip and through the use of materials which offer higher mobility of charge carriers, leading to faster response of devices and/or lower dissipation of energy as heat.

Spatial control of mobile electrons in devices is achieved by using materials in combination, forming a *material heterostructure* with bi-material interfaces as conduction barriers. At a metal–insulator interface, confinement is enforced by a huge difference in resistivity between the materials; at a semiconductor–semiconductor interface, confinement can also be enforced by proper selection of materials on the basis of electronic band structure. The exploitation of the latter physical phenomenon has become known as a bandgap engineering.

In the years ahead, the U.S. semiconductor industry faces ever greater challenges as it moves toward production of devices at feature dimensions approaching 100 nanometers. To overcome the technical barriers which loom on this path, initiatives are required to develop solutions on a broad front of science and engineering. These challenges include development of fabrication methods that are both reliable and affordable, and the search for new materials or material configurations which offer promise for device applications. Some of the potential solutions being examined have no historical precedent and, thus, represent broad interdisciplinary research issues.

On another front, an initiative has been launched in recent years by the Office of Naval Research to bring “the advantages of modularization and standardization to power electronics”. This project, which is intended to do for power distribution and control systems what the micro-chip has done for data processing, is something of a second electronic revolution. One aspect of the effort is the development of solid state switching devices based on wide band gap semiconductors (nitrides and carbides) which have relatively high thermal stability and therefore are desirable for handling large currents and voltages in power systems. Much attention has been focused on the MOS-controlled thyristor as a switching device for electronic power distribution systems, electric powered vehicles, and similar systems. Another interesting process being studied in this area is wafer bonding as a means to produce material heterostructures which cannot be grown satisfactorily by the standard vapor deposition technologies.

In many of these material configurations, stress and deformation of electronic materials are central issues to their efficient exploitation. In the sections to follow, several fundamental mechanics research topics which focus on understanding of the mechanics of electronic materials during fabrication or service at a fundamental level are described. Resolution of these issues will be important for overcoming barriers to production of electronic devices of the future.

2. Strained epitaxial materials

Semiconductor materials are used most effectively if they exist in the form of a single-crystal thin film. Many semiconductor materials with electronic properties suitable for device applications are alloys and the crystalline quality of the materials is of central importance. Films are usually grown by one of the physical or chemical vapor deposition techniques. The basic strategy for growth is to identify a single crystal of some material which is available in bulk form, which has a high degree of crystal quality, and which is of the same crystal class and orientation as the desired film. Then, using this crystal as a template, the film material is formed on it through atom-by-atom deposition. Under ideal conditions, the deposited atoms align in perfect registry with the substrate, forming a single crystal thin film with the growth template as its support. Such growth processes typically must be carried out at a temperature sufficiently high so that the deposited atoms have the mobility to search out minimum energy lattice sites; they also require ultra-clean environments to avoid chemical contamination and lattice disturbing debris.The substrate and film materials are selected on the basis of their electronic characteristics, and it is rare to find suitable material combinations which have the same lattice parameter. More commonly, there is a *mismatch* in lattice parameter between them. If the film material is to grow in perfect registry with the substrate material under such conditions, it must do so by accommodating the mismatch in lattice parameter through elastic strain. Suppose that a film of some crystal class and lattice parameter a_f grows with a nominally uniform thickness on a surface of a second (relatively thick) substrate material of the same crystal class and orientation, but with lattice parameter a_s. If the film grows with a fully coherent interface with the substrate, then it will necessarily do so with an extensional elastic strain parallel to the interface. The quantity $\epsilon_m = (a_s - a_f)/a_f$ is called the lattice mismatch parameter; it is a fundamental system parameter which, in the case of a thin uniform film on a relatively thick substrate, is numerically equal to the elastic strain in the film. Examples of unit cell dimensions at a temperature of 500°C for group IV diamond cubic materials are $a_{Si} = 0.5433$ nm for silicon and $a_{Ge} = 0.5660$ nm for germanium, and for groups III–V zinc blende cubic materials are $a_{GaAs} = 0.5658$ nm for gallium arsenide, $a_{AlAs} = 0.5664$ nm for aluminum arsenide and $a_{InAs} = 0.6062$ nm for indium arsenide. Thus, at this temperature, the elastic mismatch strain in a coherent $Si_{1-x}Ge_x$ alloy film on a Si(100) substrate is $\epsilon_m \approx -0.042x$, where x is the fraction of lattice sites in the film occupied by Ge atoms. The estimate is based on the elementary rule of mixtures, sometimes called Vegard's law, whereby $a_{Ge_xSi_{1-x}} \approx x a_{Ge} + (1-x) a_{Si}$. Similarly, for a coherent $Ga_{1-x}In_xAs$/GaAs(100) heterostructure, $\epsilon_m \approx -0.071x$. For an assumed isotropic film of thickness h and lattice mismatch ϵ_m on a relatively thick substrate, the tensile traction on any plane perpendicular to the interface is $2\mu\epsilon_m(1+\nu)/(1-\nu)$, the extensional strain in the direction of the interface normal is $-2\nu\epsilon_m/(1-\nu)$, and the elastic energy per unit area of interface is $2\mu h(1+\nu)\epsilon_m^2/(1-\nu)$ where μ is the elastic shear modulus and ν is Poisson's ratio of the film.

The stress that arises in the material due to the constraint of epitaxy has numerous potential consequences. Among these are:

(i) During processing of these materials at high temperature, the stress serves as a driving force for nucleation and growth of dislocations, stacking faults, and other defects.

(ii) The stored elastic energy provides a source of free energy to drive morphological changes, most notably evolution of irregular surface topography.

(iii) Residual stress serves as a driving force for mass transport by surface diffusion which contributes to the formation of regular arrays of epitaxial islands by self-assembly, a configuration of potential practical significance.

(iv) Elastic strain influences the electronic band structure, which is a characteristic of a periodic lattice of a certain spacing. The strain can affect the band gap of semiconductors or it can alter the relative energy in the bands, which are both important functional properties. In very small devices in which electronic transport is governed by quantum mechanical behavior, the strain can influence transport characteristics.

These phenomena will be discussed in more detail in subsequent sections.

3. Other sources of stress

In addition to the constraint of epitaxy, there are many other sources of stress in electronic materials. These arise by and large from the mutual constraint exerted by different materials on each other across shared interfaces.

A persistent problem in microelectronics is stress due to differences in coefficients of thermal expansion between joined materials. This coefficient for metals is typically an order of magnitude larger than for semiconductors or insulators. Furthermore, temperature excursions of 400°C in processing and 150°C in service are common, so that very large thermal stresses can arise to cause configurational distortion, plastic flow, delamination, buckling, film fracture and other undesirable consequences.

Controlled oxidation of semiconductor surfaces and other steps involving chemical reaction are common at the various stages in processing of semiconductor materials. Oxides are incorporated as insulating or passivating layers in devices. The formation of an oxide layer by exposing a surface to oxygen at elevated temperature can result in substantial residual stress. For example, the volume of silicon oxide formed on the surface of a crystal is nearly twice the original volume of the constituent silicon, implying substantial swelling associated with the oxidation process.

Phase transformation is yet another means for a material to respond to its environment. However, this stress related process is not very common in semiconductor materials except for the so-called surface phases where reconstruction of a lattice occurs at free surfaces to matchup dangling bonds.

There are also many less well defined sources of stress in thin-film electronic materials which appear to arise naturally during growth of a film of a specific material by means of a specific process. These are often lumped together under the heading of *intrinsic stresses*. While such stresses can be very large compared to operating stresses in engineering materials, they arise so easily because the elastic energies associated with these stresses are minuscule compared to chemical bonding energies which are recovered in forming the material. To illustrate this point, consider a material with a simple cubic lattice. For a lattice parameter of $a = 0.5$ nm and a surface energy of $\gamma = 1$ J/m^2, the chemical bonding energy per atom is about $2\gamma a^2 = 3$ eV. In contrast, if the elastic modulus of this material is $E = 10^{11}$ N/m^2, then the elastic energy per atom at a strain of $\epsilon = 0.02$ is $1/2E\epsilon^2 a^3 = 0.016$ eV, which is much less than the bonding energy. Thus, material fabrication is driven by chemical processes, and the elastic deformations which give rise to stress are carried along as secondary effects in forming a material.

4. Conditions for dislocation formation

Generally, dislocations or other defects in the semiconductor crystals which form the electronically active regions within a device are undesirable. Such defects provide easy diffusion paths for dopants which can lead to short circuits across film layers, they provide recombination centers which reduce charge carrier density, and they interfere with subsequent processing for deposition by providing sites for defect nucleation, growth or multiplication. Therefore, understanding the behavior of defects in films, with a view toward controlling them, is a major goal. The cornerstone concept of strained-layer semiconductor materials is the critical thickness concept of Matthews and Blakeslee. The concept is concerned with a strained epitaxial layer of uniform thickness on a relatively thick substrate, and it addresses the question of whether or not a strain relieving dislocation can form at a certain film thickness, lattice mismatch and Burgers vector. The most favorable site for dislocation formation is the film–substrate interface, and strain relieving dislocations in this interface are called *interface misfit dislocations*. In its simplest form, the criterion for critical thickness compares the self-energy per unit dislocation length required to form an interface misfit dislocation in a given material structure with the energy that is extracted, as the dislocation is formed, from the elastic energy reservoir stored in the film due to lattice mismatch. For small film thickness the former dominates, so dislocation formation cannot occur spontaneously in the system. For large thickness, the latter dominates so dislocation formation can proceed spontaneously in a closed system, that is, without the need for an external agent. The thickness discriminating between these two scenarios is the *critical thickness* for a given material system.

This critical thickness criterion is robust and it has been confirmed experimentally; it has become the standard for considering the stability of epitaxial thin films against degradation by dislocation formation. A good deal of research has been devoted to efforts to circumvent the critical thickness limitation on the practical use of strained layer materials in devices. One successful approach is to exploit the fact that dislocation mobility in semiconductor materials is very low compared to mobility in metals, for example. If material is deposited rapidly and at relatively low temperature, less than 500°C say, then films with low dislocation density can be grown to thicknesses well beyond the critical thickness. If such films are then covered with an unstrained capping layer and/or cooled to low temperature, they are very resistant to dislocation formation due to kinetic limitations, even though they are unstable in the equilibrium sense, strictly speaking. On the other hand, if such films are subsequently heated to a higher temperature in an annealing process, they dislocate readily.

To gain an impression of the range of parameters involved in the critical thickness criterion, consider the simplest case of a uniform film of thickness h and elastic modulus μ epitaxially grown on a substrate of thickness much greater than h but with the same elastic modulus μ. The lattice mismatch between the two materials is represented by ϵ_{m}. Aside from some dimensionless factors of order unity, the energy per unit length of a long straight strain-relieving dislocation with Burgers vector of b at the interface is $(\mu b^2/4\pi)\ln(h/b)$. In forming this dislocation, the relative slip on the glide plane is b. The traction on this plane due to the background elastic field arising from the lattice mismatch is roughly $-\mu\epsilon_{\mathrm{m}}$, so the work done by this traction in forming the dislocation is $-\mu\epsilon_{\mathrm{m}}hb$; the product $b\epsilon_{\mathrm{m}}$ is always positive. The critical thickness is defined as that thickness, h_{cr}, at which these two work contributions exactly balance each other in the closed system, or $4\pi\epsilon_{\mathrm{m}}h_{\mathrm{cr}} = b\ln(h_{\mathrm{cr}}/b)$. At a mismatch strain of 0.01, the critical thickness for dislocation formation is roughly $25b$. More complicated configurations involving compositionally graded films and compound films consisting of numerous individual layers are being investigated as a means of stress management and as a strategy for control of threading dislocation density in strained layer structures.

The foregoing discussion is based on an assessment of the energy difference between two states of a system, without concern for the *physical mechanisms* by which the system actually executes the path from one of these states to the other. An alternative approach to such questions, which is often more challenging but i usually more enlightening than the energy comparison, is to examine such mechanisms. In the case of the critical thickness calculation, the most common mechanism by which interface misfit dislocations are formed is the glide of a so-called *threading dislocation* or, more properly, a dislocation with a threading segment. If the film and substrate materials have cubic symmetry with the interface normal in the [001] crystallographic direction, say, then dislocations are likely to form by glide on the {111} planes. For example, elastic mismatch strain could be relaxed by formation of a misfit dislocation on the (111) plane; the line of the dislocation would lie along the $[1\bar{1}0]$ direction and the Burgers vector could lie along either the $[10\bar{1}]$ direction or the $[01\bar{1}]$ direction. The configuration of the entire dislocation line which produces this relaxation consists of two segments: the threading segment which extends from the free surface along the glide plane to the film–substrate interface, and the interface misfit segment which continues the line along the interface in the $[1\bar{1}0]$ direction. The length of the stationery misfit segment changes as a result of the glide of the threading segment. If the film thickness is below (above) the critical thickness, then the threading segment tends to recede (advance), thereby decreasing (increasing) the length of interface misfit dislocation. In this case, the configurational glide force on the threading segment due to the free surface, the elastic mismatch strain and the misfit segment must be determined in order to establish a critical thickness condition. For steady glide of an isolated threading dislocation, the critical thickness prediction based on configurational force is identical to that based on energy comparison, as described above.

The mechanistic picture with various configurational forces acting on the threading segment can be developed further in any of several directions. For example, kinetic rules governing dislocation motion can be adopted to investigate the *rate of strain relaxation*, as well as other aspects of the relaxation process. This is an issue of enormous practical significance. It happens that at typical growth temperatures, the time required for a threading dislocation to advance a few hundred microns or so is of the same order as the time needed to grow a film to a thickness of a few hundred nanometers. Thus, it is possible to devise a fabrication strategy by adjusting growth temperature and/or growth rate to accelerate or retard relaxation, to achieve some other objective, or to use a post-growth anneal to accomplish a particular result. In any case, a central goal is to minimize the density of threading dislocations in any particular film; threading dislocations interfere with subsequent processing and they tend to degrade electrical and optical performance of materials.

While critical thickness is characterized by the spontaneous growth of a single threading dislocation, significant macroscopic strain relaxation requires the formation of many interface misfit dislocations, each laid down by the glide of a threading dislocation. Thus, work toward understanding *dislocation interactions* provides a host of challenging mechanics problems in this area. As an interface misfit dislocation is formed by the motion of a threading dislocation, elastic strain is relaxed along its path. This is a very localized effect, however, extending only a few times the film thickness off to either side of the path. Thus, other dislocations form on parallel glide planes at some distance from each other. As the film thickness increases through growth, the mean spacing of such parallel dislocation arrays diminishes in a predictable way.

The possible orientations of the misfit dislocations are limited by the the crystallography of the system. For example, for diamond cubic structures (silicon, germanium and their alloys) or cubic zinc blende structures (gallium arsenide and other III–V compounds) with the interface normal coinciding with a cube edge, dislocations form in two parallel arrays with the members of one array being perpendicular to the members of the other. The influence of misfit dislocations formed earlier in the relaxation process on the progress of a gliding threading dislocation formed later is of great practical significance. To a large extent, this interaction determines the ultimate density of threading dislocations in a material structure, as well as a final residual elastic strain in these structures.

Another approach being pursued actively to extend the practical range of strained thin films beyond the critical thickness barrier is the use of *compliant substrates* for film growth. The central idea is that, if single crystal substrates are used which are roughly as thick as the films to be grown on them, then both the film and substrate will share in the accommodation of mismatch strain. This could reduce the residual elastic strain in the film significantly. Furthermore, by selecting materials and dimensions carefully, it may be possible to force dislocation formation, once it eventually occurs, into the substrate rather than in the film, thus leaving the film surface unaffected. The theoretically predicted advantages to be gained by substrate compliance are very significant. A serious practical limitation arises, however, by the need to actually support such a system; a film–substrate system 1 cm in lateral extent but only a few hundred nm thick cannot exist without being supported in some way on a solid base, or handle wafer. Thus, the actual degree of compliance permitted by the handle wafer becomes a critical issue. The most promising strategy being pursued is to form a structure with an amorphous thin layer between the compliant single crystal substrate, on which the film is to be grown, and the handle wafer. The most common materials being examined for this purpose are amorphous silicon, silicon oxide, and silicon oxide doped with boron or phosphorus. The basic idea is that the amorphous layer will flow as a viscous medium during processing and, thus, permit a certain degree of compliance on the part of the substrate. While some data are available to indicate promise for the configuration, it has not yet been developed into a production technology. It continues as an area of active research which relies on a clear experimental demonstration that the expected level of compliance can be achieved. Just the pre-growth process of forming the configuration of a 100 nm single crystal film on a 100 nm oxide layer on a handle wafer is fraught with difficulty.

5. Stress-driven surface evolution

A characterizing feature of a homogeneous elastic body is that there is a well-defined *reference configuration* to which it returns when all applied loads are removed. While typically viewed as being immutable, there are circumstances under which the shape of the bounding surface of the body in this reference configuration can change over time as, for example, in condensation/evaporation or diffusion processes. As noted above, condensation is a physical process which is central to making high quality semiconductor materials for microelectronic applications. Furthermore, many temperature cycles are involved in the various steps required for manufacture of complex devices. The focus here is on the particular change-of-shape mechanism of mass transport by surface diffusion. Mass rearrangement typically preserves crystal structure in single crystal films, so that there is a well defined reference configuration at any time.

Mass transport by stress-driven diffusion is typically slow, and it can occur to a significant degree only when the process under consideration has the features of relatively high stress, high temperature and small size scale. These features are characteristic of strained-layer semiconductor material systems, of course, for which the magnitude of stress can exceed a gigapascal, the materials are grown or processed at temperatures of 500–600°C, and submicron physical dimensions are typical.

A consequence of the internal stress is that the materials under consideration are deformed, in general, and the processes are sufficiently slow so that they are always in mechanical equilibrium. They are not necessarily in thermodynamic equilibrium, however, so they tend to evolve in time in such a way as to decrease the system free energy. The surface field representing the tendency for the system to change the shape of its reference configuration is the *chemical potential field*. Under circumstances for which this change can arise only through mass transport over the surface of the material, the chemical potential at a point on the surface is defined as the increase in Helmholtz free energy (isothermal potential energy) of the system due to addition of one unit of mass (one atom or one unit volume) at that point on the surface at the prevailing local strain. The basic idea is that, if the chemical potential is lower in some region than in an adjacent region, material will diffuse toward the region of lower chemical potential, thereby lowering the free energy of the system. In general, material tends to diffuse against the chemical potential gradient along the surface. Actually, thermally activated atoms diffuse randomly in huge numbers in all directions on the surface of a heated crystal. A gradient in chemical potential induces a slight bias to this process which is perceived macroscopically as mass transport.

It was recognized above that the chemical forces involved in a material are orders of magnitude greater than the mechanical forces when the two are compared on an equal basis. Nonetheless, it appears that stress can play a role in diffusion in cases where the gradients of chemical forces are very small. The reason for this can be understood by considering the common local form of the surface chemical potential. Aside from constant factors, this quantity at a point on the surface is $U-\gamma\kappa$ where U is the local strain energy density, γ is the local surface energy density and κ is twice the mean curvature of the surface which may be positive or negative. The sign convention followed is that a principal curvature at a point on the surface is positive (negative) if the center of curvature lies on a normal line running out of (into) the material from that point. Even though surface energy typically is much larger than elastic energy on a ‘per atom’ basis, its effect is diluted by the curvature. For example, if γ is two orders of magnitude larger than U on this basis, then a surface radius of curvature of one hundred atomic spacings renders the two contributions to the chemical potential to be of the same order, and thus in competition.

The chemical potential is defined as a function of position on the surface in terms of deformation and surface shape, under the assumption that the free energy of the system can change only as a result of a change in net surface area or net elastic strain energy of the material. It is well-known that the flat surface shape is stable under small perturbations in shape as long as the surface energy density had a positive value. The reason is that any change in shape results in more surface area, and therefore greater surface energy. In the presence of stress, the elastic energy of a body with a flat surface *always diminishes* if the surface becomes wavy. Thus, this effect counteracts the effect of surface energy, and it immediately raises the possibility that the flat surface shape is unstable under small perturbations in shape if the reduction in elastic energy more than offsets the corresponding increase in surface energy. To see this in a more mechanistic way, assume that mass rearranges itself by surface diffusion so as to reduce the total free energy. For a stressed material with a wavy surface, mass will tend to flow from the valleys where the stress is concentrated toward the peaks where stress is low in order to reduce the elastic energy contribution to the free energy, represented by U. On the other hand, it will tend to flow from the peaks to the valleys in order to flatten the surface and thereby to reduce the surface energy contribution. The relative strengths of these effects determines the stability of a configuration. The general finding is that the flat surface is stable if the wavelength of the perturbations is smaller than some critical value, but unstable if the characteristic length is greater than this value. The critical wavelength which discriminates between stability and instability is proportional to the ratio of the surface energy density γ to a reference elastic strain energy, say modulus × mismatch strain squared or U_m, as must be so on dimensional grounds alone. This length scale $\ell = \gamma / U_\mathrm{m}$ is a system parameter. Any real surface includes imperfections with a wide range of wavelengths, and the wavelength of most interest is the one which corresponds to the highest rate of growth in amplitude.

At first sight, the conclusion that all perturbations in shape with wavelength above some critical value are unstable may seem peculiar. This critical wavelength for a mismatch strain of about 0.01 or one percent is roughly one-half micron. The shape of any real object is imperfect, of course, so the apparent implication is that the configuration of any large stressed solid object will evolve over time. The key to resolving this paradox is the role of time in the process. Any system with shape evolving by stress-driven diffusion is characterized by the natural length $\ell = \gamma / U_\mathrm{m}$. Here, γ is the surface energy density and U_m is a reference elastic energy density. During surface diffusion, the rate at which the shape evolves is determined by the temperature, diffusivity and this length scale. Of particular note for present purposes is that the *characteristic time* for surface diffusion depends on this natural length scale according to ℓ^4. An implication of this observation is that morphology evolution is not expected to occur on macroscopic size scales.

A particularly fascinating small material structure of significant practical interest is a *strained epitaxial island* residing coherently on the surface of a substrate. It was noted above that, in the presence of a substantial elastic mismatch strain, the surface of a thin film on a substrate tends to become wavy. If the mismatch is large enough, the valleys of surface waviness deepen and eventually reach the substrate, thereby isolating individual clusters of film material; these clusters are called islands.

Proper description of the behavior and interaction of such islands poses a challenging and complex set of problems. As the volume of an isolated island increases, its free energy per unit volume diminishes and it tends to assume shapes with ever increasing height-to-width aspect ratio. As the elastic energy stored in an island increases with increasing size, strain relieving dislocations tend to appear in the interface which, in turn, causes the island aspect ratio to diminish. Concerning interaction of islands in close proximity, the dependence of free energy per unit volume on volume noted above implies the existence of an energetic driving force for larger islands to absorb smaller islands which have higher free energy, thereby causing the island population on the surface to coarsen.

While this coarsening argument is generally correct, the tendency to coarsen the array is not always evident in observations of the behavior of *arrays of islands*. Instead, through their interactions, the islands tend to *self-organize* into regular arrays with a narrow range of island sizes. The reasons for this outcome are not yet completely understood, but several important factors which seem to bear on the outcome have emerged. For one thing, islands tend to repel each other upon approach by interacting through the substrate. In effect, any island perceives the presence of a nearby island as an apparent increase in the stiffness of the substrate, thus increasing its own free energy. The repulsive configurational force between islands is proportional to this change in energy with respect to the separation distance.

A second important factor concerns the rate of the process by which one island absorbs another. If islands in close proximity are very different in size, then there is a strong gradient in chemical potential from the larger to the smaller and, therefore, a relatively high rate of diffusive mass flux from the smaller to the larger. On the other hand, if the islands are identical in size and shape then, by symmetry, the rate of diffusive mass flux between them is zero. Thus, regular arrays of islands of more-or-less the same size are far more persistent than irregular arrays, although they are still not stable arrays. Currently available evidence points to these two factors as being largely responsible for the process of self-organization of regular arrays of epitaxial islands.

The practical interest in epitaxial islands stems from the fact that these natural structures provide the most promising means by far for fabrication of *quantum wires* and *quantum dots* as active regions in ultra-small devices. Such structures offer major improvements in size reduction and electronic characteristics. Just as with large arrays of transistors in memory chips, the regularity of the array is essential to achieving predictable properties which fall within fairly narrow bounds for actual values. The alternative to formation of such arrays by natural self-organization is to fabricate such structures by a means of lithographic methods from uniform strained layer structures. The spatial resolution required rules out most standard fabrication methods based on optics and chemical etching, so the fabrication costs become prohibitive. Because of the promise of these small structures for practical applications, the role of mechanical effects on the performance of devices fabricated from these small structures is considered in the next section.

6. Influence of strain on electronic properties

The electrical transport properties of a doped semiconductor material are established by the periodicity of the crystal lattice. A uniform elastic strain imposed on the lattice produces an energy shift in the band structure. Electrical transport through a device consisting of a strained epitaxial heterostructure is affected by this shift. The magnitude of a uniform strain field affects the amount of electron or hole current per unit area of conduction cross section, but this effect should be independent of the conduction cross sectional area. Furthermore, the *spatial distribution* of electron or hole charge density at a given applied voltage should remain independent of the conduction cross sectional area. Recent observations indicate, however, that as lateral dimensions of devices are reduced into the submicron range, this simple scaling idea breaks down; the current per unit cross sectional area and the spatial distribution of charge density are affected. A likely explanation for this observation is that the deviations are due to the influence of nonuniform elastic strain in small heterostructures.

To make the discussion a bit more concrete, consider a quantum device in the configuration of a layered right circular cylinder. The cylinder is epitaxially bonded to a silicon substrate at one end, and it consists of a stack of circular disks in the order SiGe/Si/SiGe/Si/SiGe. This structure has actually been formed by growing thin films sequentially in the indicated order, and then removing all material except for the isolated composite cylinder by lithographic processing. The inner most silicon germanium layer in the stack is a quantum well, isolated by the silicon layers as barriers on either side. The total current flow through the cylinder, driven by an applied voltage of given magnitude, is governed by the charge density in the silicon germanium quantum well layer. The charge density in the quantum well layer is independent of cross sectional area if the strain is uniform. Observations indicate, however, that features of the total current as a function of applied voltage change with decreasing cylinder diameter for diameters below about one micron.

When the epitaxial films are deposited initially, the strain is uniform except near the remote outer edges of the films. The subsequent process of isolating the cylinder produces free lateral surfaces on which traction had previously acted. The free surfaces allow for elastic relaxation of the mismatch strain in the cylinder, and the degree of relaxation increases as the diameter is reduced because the free surface effect is more pervasive. Furthermore, the relaxation results in a *nonuniform* strain distribution in the quantum well, and the degree of nonuniformity increases as the diameter is reduced.

The partially relaxed, nonuniform strain fields lead to novel electronic properties in devices like the layered circular cylinder. The strong relaxation effect in smaller cylinders results in large energy band shifts. In some devices, these energy shifts are significant because the semiconductor band gap is affected. In the layered cylindrical structure, the nonuniform strain induces localization of charge density, or *confinement*, which is an important effect in producing the next generation of quantum semiconductor devices.

These strain effects are amenable to analytical interpretation at several levels. From a continuum perspective, for example, the residual strain in the heterostructure can be determined independently of the electrical and transport properties of the material by means of standard finite element analysis. This strain induces a nonuniform potential field which affects the behavior of charge carriers in the heterostructure. The nonuniform potential must be included in the Schrödinger equation governing the wave function of the charge carrier. Then the influence of strain on transport relies on the interpretation of the strain effect on the charge carrier wave function and its energy spectrum. Alternatively, from an atomistic perspective, the residual strain field and the electronic properties can be treated as coupled. The energy band structure and the strain field at a given position in a heterostructure are then determined simultaneously in a self-consistent quantum mechanical atomistic calculation. The electrical transport properties of the material follow from an interpretation of the local electronic properties of the heterostructure.

This general area of semiconductor quantum structures is emerging as a major focus in materials science and device fabrication because of the insight to be gained concerning the properties of materials and the potential for development of practical devices with unprecedented characteristics. The small structures are invariably strained due to their composition and fabrication methods. As was noted in the previous section, mechanics research has a role to play in understanding the formation of these small structures. In the years ahead, it is likely that mechanics research will also play a central role in understanding the electronic performance of these structures because of this coupling between strain and transport properties of materials.

7. Summary

The foregoing discussion is intended to provide a general framework for discussion of research issues in the area of mechanics of electronic materials. There are a number of specific contemporary research problems in this area for which broadly based solutions will have immediate impact on the evolution of technology. The area is highly interdisciplinary, and solving these problems will hinge on cooperation between researchers in mechanics, materials science, condensed matter physics and electronics. Among the questions which are likely to be addressed over the next decade are:

- During elastic strain relaxation in epitaxial heterostructures with mismatch beyond critical thickness, how do dislocation interactions influence the process? Is there a more direct means of controlling threading dislocation density in films?
- Are there advantages to be gained from using compositionally graded epitaxial films or multilayered films as a means of stress management in heterostructures?

- How should the process of stress-driven surface morphology evolution be described to properly account for chemical segregation or alloy decomposition during the diffusion process?
- What are the principal factors which control the size and relative position of epitaxial islands as they are formed on a substrate during fabrication of quantum structures?
- How can the rate-dependent strain relaxation in a thin amorphous layer be measured or otherwise characterized to guide the development of compliant substrate systems? Can these buried amorphous layers be used to absorb dislocations from adjacent crystal films?
- What is the role of surface crystal facets and facet junctions in the growth of epitaxial islands? How does strain affect faceting?
- What is the influence of mechanical strain on the electronic characteristics and transport properties of small quantum structures being developed for device applications?

Other important research areas could also be discussed under the heading of mechanics of electronic materials. Among these are metallization and interconnect technology in integrated circuits; wafer bonding as a means of forming particular heterostructures without relying on vapor deposition; delamination and fracture of thin films, particularly interfacial fracture in complex multi-layered systems; and the influence of chemo–mechanical polishing on mechanical properties of dielectrics and other materials. Each of these areas provides challenges for mechanics researchers.

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Further reading

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