10 SCIENTIFIC HIGHLIGHT OF THE MONTH

Ideal strength of nano-structured components

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Abstract

The ideal (theoretical) strength was originally defined as the stress or strain at which perfect crystal lattice became mechanically unstable with respect to arbitrary homogeneous infinitesimal deformation. This has been intensely investigated because the ultimate strength without defects is a fundamental mechanical characteristic of materials. In the analyses, the instability criteria have been studied on the basis of elastic constants. Recent developments in computational technology make it possible to analyze the ideal strength on the basis of quantum mechanics. On the other hand, it is well known that the mechanical strength of components is dependent not only on (1) material (atom species), but also on (2) loading condition and (3) structure. Because most studies on the strength in terms of atomic mechanics have focused on the factor (1) (materials), analysis has mainly been conducted on simple crystal consisting of perfect lattices (*e.g.* fcc and bcc) under simple loading conditions (*e.g.* tension), though some have explored the properties of bulk materials with defects (*e.g.* vacancy and grain boundary). Small atomic components (nano-structured components) such as nano-films, nano-wires (tubes) and nano-dots (clusters) possess their own beautiful, defect-free structure, namely ideal structures. Thus, they show characteristic high strength. Moreover, utilizing the structure at the nanometer or micron level is a key technology in the development of electronic devices and elements of micro (nano) electro-mechanical systems (MEMS/NEMS). Therefore, it is important to understand the mechanical properties not only for the sake of scientific interest, but also for engineering usefulness such as design of fabrication/assembly processes and reliability in service. In the other words, the effects of structure (factor (3); *e.g.* film/wire/dot) have to be understood as the basic properties of atomic components. Thus, the definition of ideal strength should be expanded to include the strength at instability of components with ideal structures under various external loads (factor (2)), which provides fundamental knowledge of nano-structured materials. In this paper, we review works on the strength of ideal nano-structured components in terms

of factor (3), mainly under tension and discuss the strength criterion of arbitrary atomic structure/material under arbitrary loading.

1 Introduction

The ideal strength (theoretical strength) was originally defined as the stress or strain at which perfect crystal lattice became mechanically unstable with respect to arbitrary homogeneous infinitesimal strain (*e.g.* [1]). It has been intensely investigated because the ultimate strength without defects is a fundamental mechanical characteristic of materials. However, it is well known that there is an eminent difference between the ideal strength and the actual one observed experimentally, and this fact led researchers to the discovery of dislocation which plays important role in crystal plasticity. Because the ideal strength physically means the maximum resistance against the external stress (strain) that the material possesses, such high strength was experimentally observed in only whisker that included few defects. Recently, the strength obtained by nano-indentation is attracting researcher's attention because the extremely localized evaluation reveals properties in a defect-free region (*e.g.* [2,3]).

On the other hand, investigation of the strength of bulk materials and macroscopic structures has long history (*e.g.* [4]), and the number of related articles published runs into astronomical numbers. The key point derived from the experiences is that the mechanical strength of components depends not only on (1) materials (atom species), but also on (2) loading conditions (mechanical boundary conditions) and (3) structure. Although the environmental effect is also prominent, it lies outside the scope in this article. The interactions among those factors complicate the fracture phenomenon, and this is one of the main reasons why it is difficult to understand the "strength" of materials.

(1) Material The ideal strength gives a fundamental insight into factor (1). In early analyses, the focus was on the simple structure of perfect crystal (*e.g.* fcc and bcc) under simple loading conditions (*e.g.* tension) because it was difficult to correctly calculate the interactions among the atoms. In other words, the inter-atomic potential was not reliable for the crystal lattice with complex structures under high strain conditions. The precise analysis became possible in this decade due to the progress in computational resources and the technique for simulating quantum mechanics.

(2) Loading The homogeneous deformation of a crystal is represented by the change in shape of a unit cell, namely the strain, which is the symmetric second order tensor, ε_{xx}, ε_{xy}, ε_{xz}, ε_{yy}, ε_{yz}, and ε_{zz}. Of course, it can be related to the homogeneous stress tensor through proper constitutive equations. At first, researchers were interested in the strength in uni-axial tension; however, the ultimate strength should be understood as a function of the combination of strain components in general. For example, the strength under the shear along the slip direction of the crystal gives us fundamental knowledge of the dislocation nucleation and glide.

(3) Structure The strain tensor can not fully describe the deformation of a crystal when the unit cell includes many atoms, *e.g.* a perovskite structure. That is, the inner displacement plays important role in the deformation [5], signifying that the structure has a strong influence on

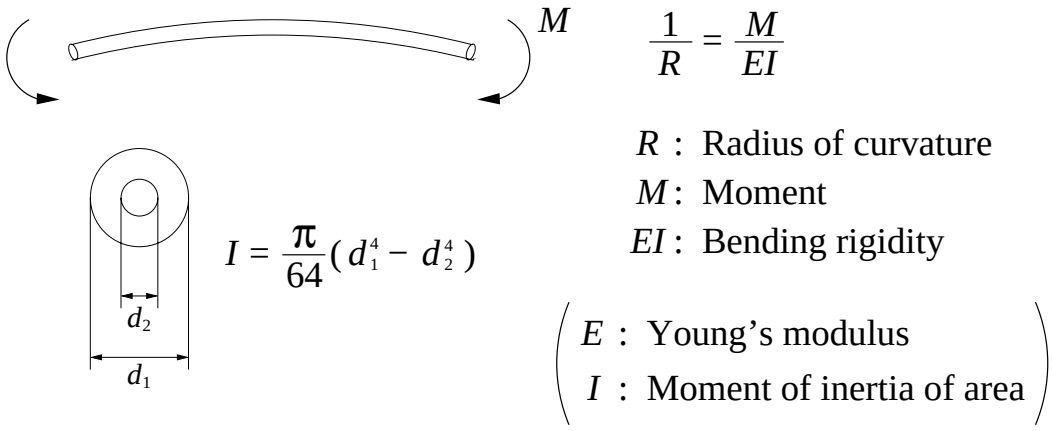


Figure 1: Bending of a tube. The rigidity is dependent on the configuration of tube (the moment of inertia of area).

the strength at the atomic scale. Since we intend to discuss the strength of nano-materials that usually possess characteristic atomic structures, the instability of complex structures becomes a crucial factor in the analysis. In terms of factor (3), we can gain valuable suggestions from the conventional cognition in the mechanical engineering approach on the basis of the continuum mechanics concept. For example, it is well known that the shape of component strongly influences its rigidity and structural strength. The rigidity of the tube illustrated in Fig.1 is determined by the shape of the cross-section (diameter and wall thickness) as well as its elastic coefficient. This, of course, basically represents the carbon nano-tube, which is a typical nano-structured component. Thus, it implies that the structural factor becomes essential, although factor (3) has not been discussed well in past analysis of ideal strength.

In the context of structural analysis, over last decade multi-scale simulation is spotlighted as an *ad hoc* method connecting molecular dynamics to continuum mechanics. However, it is necessary to identify the representative indicator for characterizing the strength of nano-structured materials as fundamental knowledge. Small atomic components such as nano-films, nano-wires (tubes) and nano-dots (clusters) possess their own beautiful, defect-free structures, namely the ideal structure. Consequently, they display characteristic high strength. Moreover, utilizing the structure at the nanometer or micron level is a key technology in the development of electronic devices and elements of micro or nano electro-mechanical systems (MEMS or NEMS). Their complex systems can be decomposed into elements with simple configuration such as the film, wire and dot. For this reason, it is important to understand the mechanical properties not only for the sake of scientific interest but also for engineering applicability such as design of fabrication/assembly processes and reliability in service. As the basic property of component, the effects of structure (factor (3); *e.g.* film/wire/dot) and the loading condition (factor (2); *e.g.* combined load of tension/shear) on the ultimate strength have to be understood. In particular, analysis of instability of component with an ideal defect-free structure gives fundamental insight into the strength of atomic structure. In other words, the definition of ideal strength should be expanded to include the strength at point where nano-structured components with ideal structure (factor (3)) become unstable under various boundary conditions (factor (2)).

Many attractive materials with the ideal structure have been reported not only in scientific journals [6] but also in books (*e.g.* [7-11]; in this series of highlights, there are excellent reviews as well [12, 13]). However, it is not our aim here to review them. We do, however, select some examples investigated by the auth's group, and present characteristic behavior of their strength in Section 2. In terms of the strength, it is clear that mechanical instability under external load or displacement is essential for the analysis of nano-structured materials. Thus, in section 3 we explore the instability criterion.

2 Strength of material with ideal structure

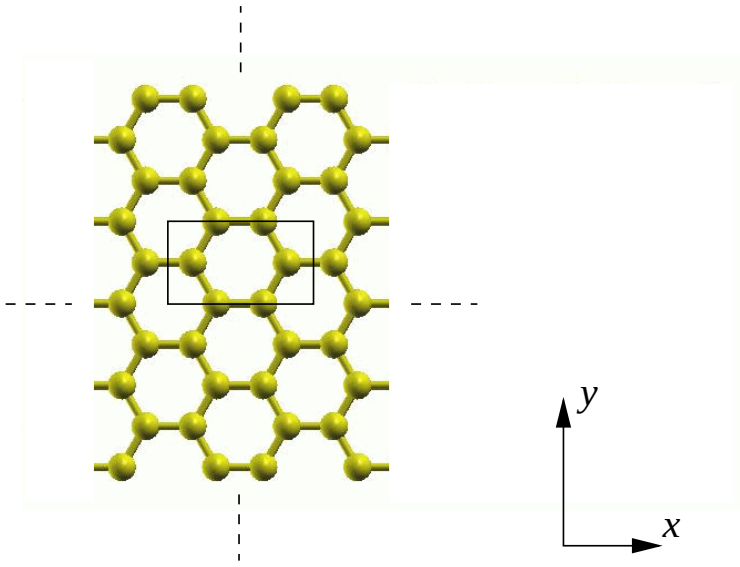
To analyze an "ideal" bulk crystal, the three-dimensional periodic boundary condition was applied to the unit cell. Neglecting one- or two-dimensional periodicity, we can easily obtain typical nano-structured components without defect inside. The periodicity is held in the clean structure, though it is low-dimensional. Thus, there are two-dimensional and one-dimensional materials with ideal structure referred to as "ideal" film and "ideal" wire (or tube), respectively. In this context, the cluster (nano-particle) and the fullerene (cage-like structure) should be classified as zero-dimensional ideal structures.

2.1 Two-dimensional structure

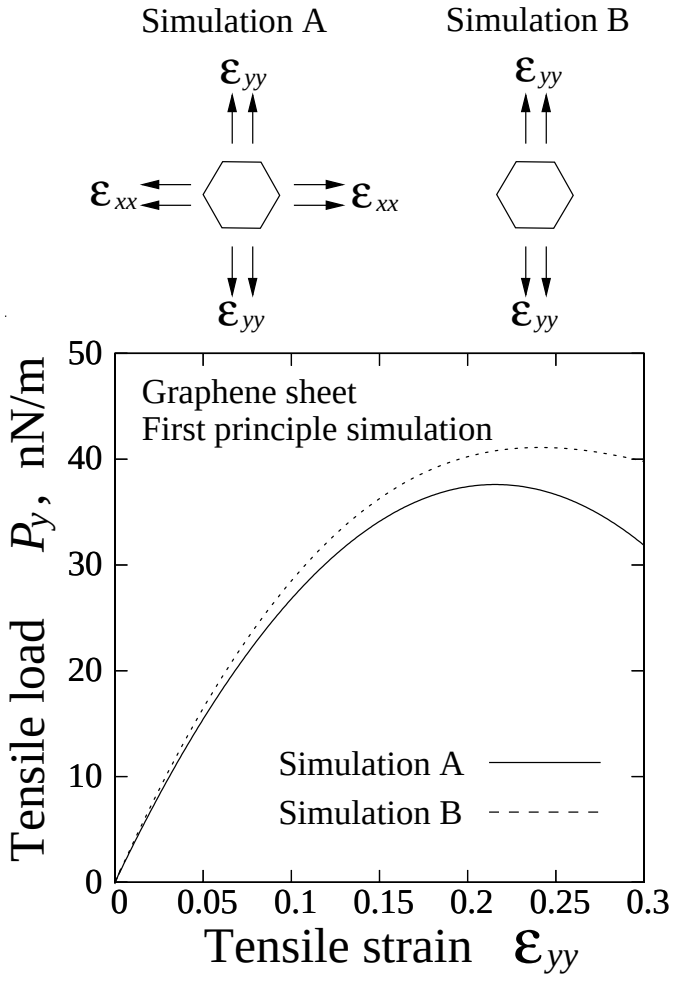
Graphene sheet When the "ideal" film (film with ideal understructure) is defined as the structure with the perfect two-dimensional periodicity, the simplest one is a layer of the graphene sheet which consists of a hexagonal carbon network as illustrated in Fig.2 (a) [14-18]. It is an absolute mono-layer film, for which the unit cell is indicated by the solid square in Fig.2(a)[14]. The equi-tensile strains, ε_{xx} and ε_{yy}, (Simulation A) or the uni-axial tensile strain, ε_{yy}, (Simulation B) are applied to the cell under the constraint condition that the other strain components are kept null [14]. The dotted and solid lines in Fig.2 (b) show the relationships between the load P_y and the strain ε_{yy} along the y-axis, respectively, analyzed by first-principle simulation (LDA, plane-wave basis, norm-conservative pseudopotential). Although it is easy to convert the load into the stress to evaluate the thickness from the distance between layers of stacked graphene sheet, we prefer to represent it here without the conversion in order to avoid ambiguity. This provides fundamental knowledge on the strength of nano-structured carbon such as fullerenes, nano-tubes, hones and so on. Moreover, the ideal strength, which is given by the peak load, in the uni-axial tension is higher than that in the equi-axial tension. Thus, the ideal strength is dependent on the combination of external strains (loading condition).

By comparing the load-strain curves, we can examine the validity of classical potential (*e.g.* the Brenner potential [19]) and the tight-binding (TB) method [20] under the high-strain condition. The result obtained by TB showed excellent correspondence with that in the above first-principle analysis, whereas the Brenner potential does not.

Thin film with reconstructed surface The development of high-vacuum technology enables us to procure well-defined surfaces, and extensive investigations have been devoted to exploring the structure at the surface as well as exotic properties stemming from it. The lattices near

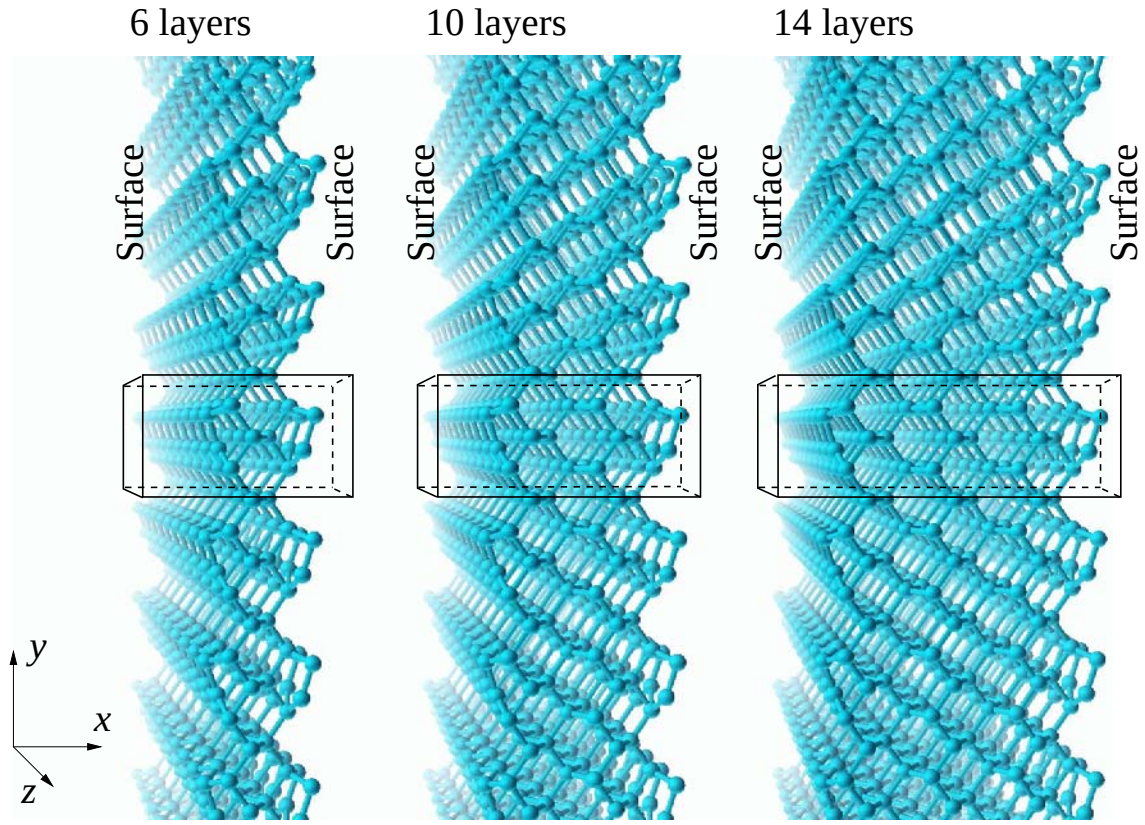


(a) Ideal structure of carbon layer in graphene sheet and the unit cell for calculation.

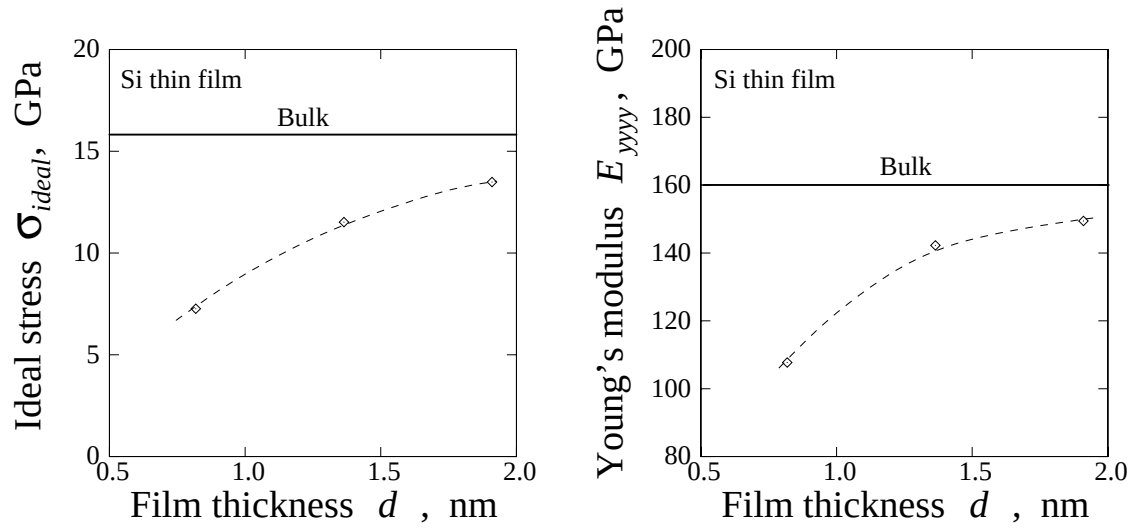


(b) Relationships between the load and the strain under tension.

Figure 2: Strength of graphene sheet [14].



(a) Ideal structures of thin films with 6, 10, 14 silicon layers, and their unit cells.



(b)Dependence of ideal strength and elastic coefficient on the film thickness.

Figure 3: Strength of silicon thin film[26].

the surface are relaxed and they sometimes form notably different structures from those in the bulk. In particular, the first layer shows a unique structure due to the reconstruction when the atoms on the surface have dangling bonds (*e.g.* [21-24]). Since the thin film is interpreted as being a material sandwiched by the surfaces, the mechanical property reflects the nature of the surfaces. In the other words, we may be able to determine the Ideal structure of carbon layer in graphene sheet and the unit cell for calculation.we may be able to determine the ideal surface effect on the strength by comparing the strengths between the bulk and the film [25].

Here, we show the strength of a silicon thin film with the excellent reconstructed surface of (100), of which the simplest structure is 2×1 illustrated in Fig.3 (a), as an example of an ideal film [26]. The freedom of a periodic cell in a film depends not only on the crystal structure but also on the thickness. We prepare a calculation cell of silicon with several thicknesses, and apply the uni-axial tensile strain, ε_{yy}, to the cell under the free transverse-stress condition, $\sigma_{xx} = 0$ by the first-principle simulation (GGA, plane-wave basis, ultrasoft pseudopotential).

Figure 3 (b) shows the dependence of the peak tensile stress and the elastic coefficient, E_{yyyy}, on film thickness. The figure indicates that the peak stress increases as the film thickens [26], and approaches the ideal bulk strength (thick line). It also reveals softening in the thinner film, signifying that the surface inherently possesses a weakening effect. However, the magnitudes of strength and the elastic coefficient, E_{yyyy}, of a 2-nm-thick film reach about 90% of those of the bulk. This implies that the surface property dominates only a region of less than 1 nm deep.

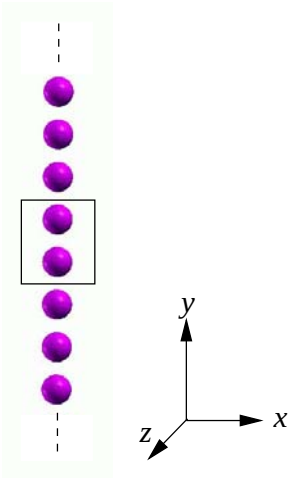
2.2 One-dimensional structure

There are several types of ideal wire with perfect one-dimensional periodicity, such as atomic chains, solid wires and tubes (hollow ones). In this section, we will present a typical strength analysis of them.

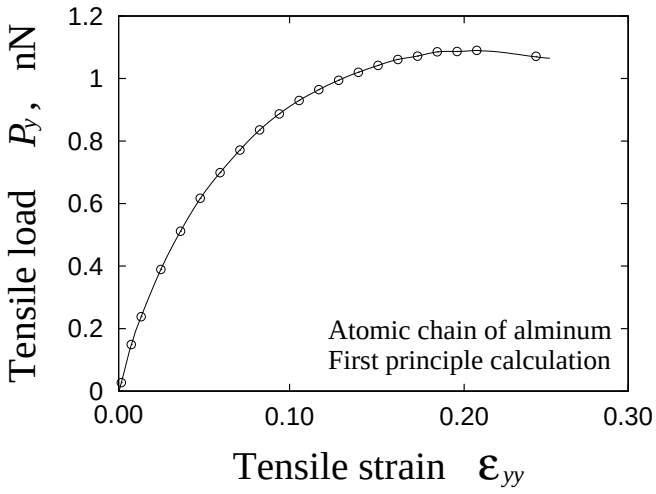
Atomic chain In recent years, it has become possible to arrange atoms in order by employing a sensational manipulation technique. An atomic chain is the simplest wire. It can be experimentally created and be observed *in situ* by an electron microscope (*e.g.* [27]). Figure 4(a) illustrates the atomic chain in which atoms align in a string [28-31].

Numerical simulation (LDA, plane-wave basis set, and norm-conserving pseudopotential) is conducted on the calculation cell of an aluminum atomic chain shown by the dotted square in Fig.4(a)[30]. The result reveals that the equilibrium interval of atoms is much shorter than the closest distance between atoms in the bulk fcc crystal of aluminum. A tensile strain is then imposed on the cell. The load-strain curve shown in Fig.4 (b) indicates a strength of 1N and a critical strain of 0.2. One way of perceiving the chain's strength is to compare it with the bulk providing that the fcc crystal is a bundle of atomic strings as illustrated in Fig.4 (c). Not only is the failure load of the atomic chain much higher than the critical tensile load per string in the bulk, but the elongation is eminently lower [30]. Therefore, we notice that the chain is more brittle than the bulk crystal.

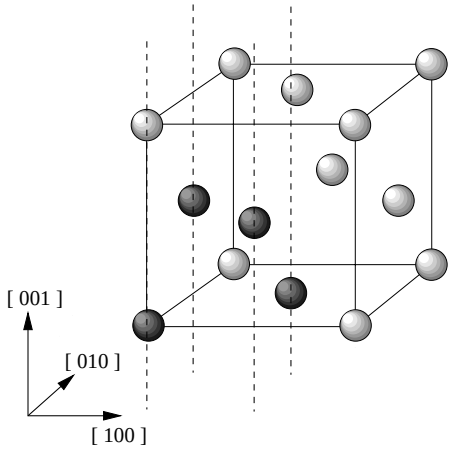
Nano-wire There are two types of structure that form an ideal solid wire. One is a crystal with an ordinary structure surrounded by surfaces, and the other is a very thin wire with an exotic structure, namely a nano-wire. For the former, a similar property as shown in thin film



(a) Illustration of atomic chain and the calculation cell.

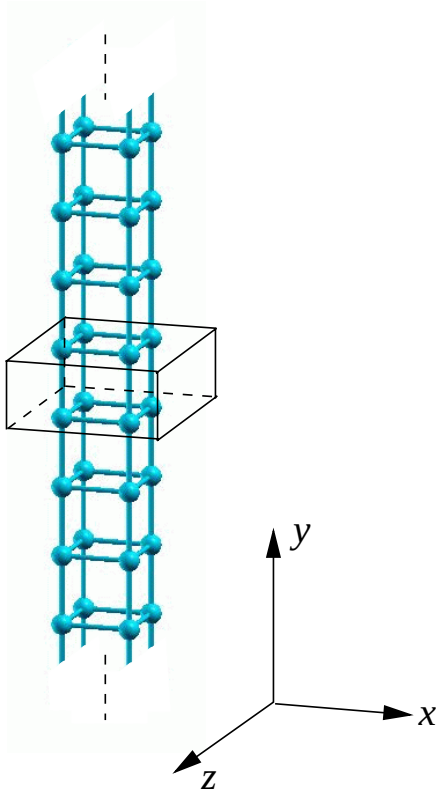


(b) Relationship between the external load and the strain under tension.

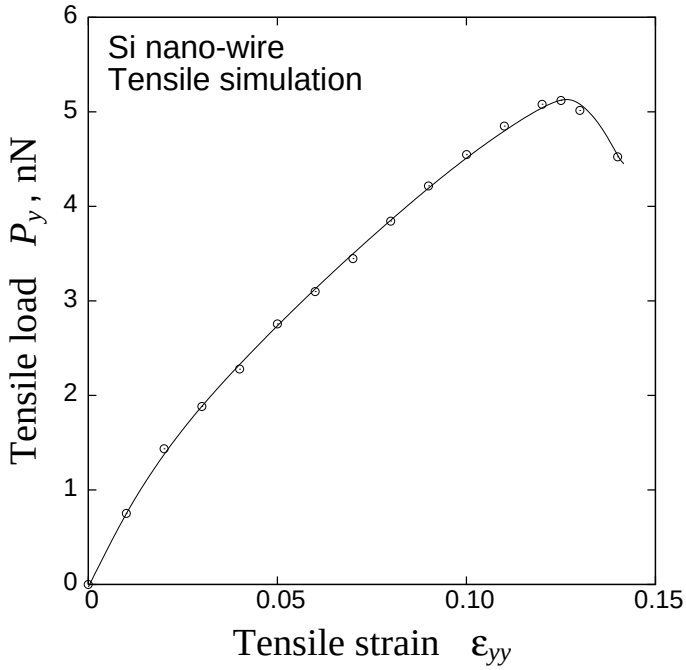


(c) Illustration of virtual strings in the fcc crystal.

Figure 4: Strength of aluminum atomic chain[30].



(a) Ideal structure of silicon nano-wire and the unit cell.



(b) Relationship between the external tensile load and the strain.

Figure 5: Strength of silicon nano-wire[26].

(Fig.3 (b)) is readily conceived. The wire becomes softer and weaker as the diameter shrinks to the extent that it possesses the structure of a crystal lattice.

In the meantime, since the extraordinary structure in the latter [32-38] still holds its periodicity along the wire axis, it should be categorized as an the ideal wire as well. Figure 5 (a) shows an example of the nano-wire structure proposed for silicon [26].

Tensile behavior of the unit cell marked by thick squares in the figure is simulated by the first-principle method (GGA, plane-wave basis set, and ultrasoft pseudopotential) [26]. The relation of load versus strain is shown in Fig. 5 (b), indicating the peak strength of about 5 N. However, care is necessary since the wire possesses various meta-stable structures due to loose constraints imposed by neighboring atoms. This requires strict judgment of instability as discussed in section 3.

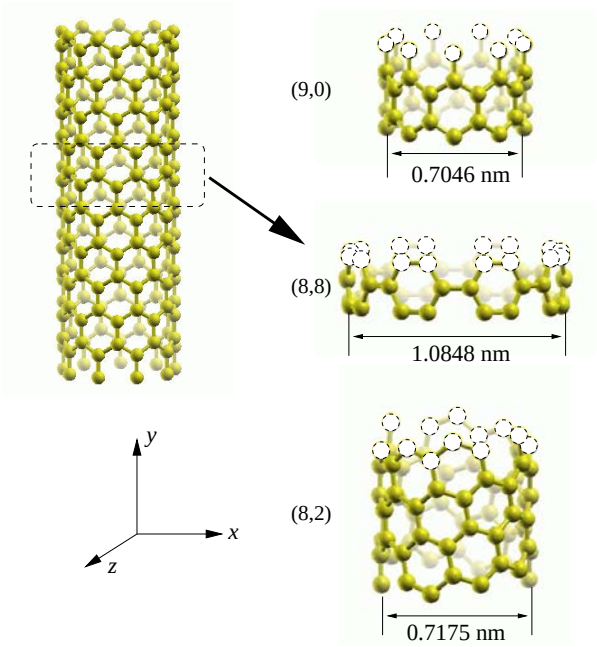
Tube Since the discovery of fullerene, intensive research attention has been directed foward materials with hollow structures at the nano scale. As a wire, the carbon nano-tube (CNT) possesses beautiful tubular structure with rich properties, that have been rigorously investigated both experimentally and theoretically (*e.g.* [39-47]), promising potential use in future miniature devices and machines.

Figure 6 (a) shows the unit cells of CNT with different chirality which represents the understructure of the tube. They have a similar diameter of 0.7-1.0 nm, and tensile simulation is carried out based on the TB method [46]. Here, (9,0) and (8,8) are known as Zigzag and Armchair types, respectively. Referring the graphene layer shown in Fig.2 (a), the strength of CNT (8,8) can be compared with that of raw material. (In the case of Fig.2 (b), the transverse strain is constrainted. For exact comparison, the simulation of the graphene layer should be conducted under the free transverse-stress condition.) This signifies the small effect of curvature on the strength. The effect of chirality can be determined in a similar manner.

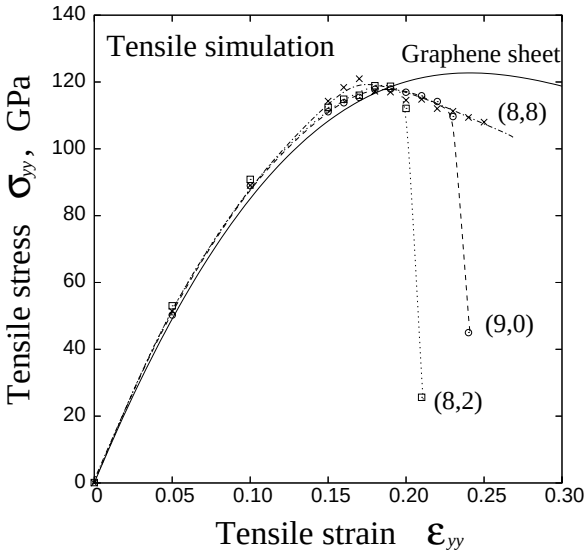
The tensile curves shown in Fig.6 (b) reveal that the Armchair type shows higher critical-stress than the Zigzag type though there are few differences among CNTs with different chirality. The stiffness at the equilibrium (no external load) is also only slight dependent on the understructure. Applying an unbalanced load (strain) to the side wall of CNT as shown in Fig.6 (c), we can analyze the effect of pure bending. Since this provides fundamental knowledge of defect-free nano-structure components under simple loading, it also should be included in ideal strength, though the one-dimensional periodicity along the y-axis is lost. At this point, the instability criterion of an arbitrary structure under an arbitrary external load becomes crucial in the analysis. In general, CNTs inherently possess various shapes including bent tubes, hones, and so on. The strength of typical ones, which provides fundamental comprehension and insight into the strength of the various CNTs, should be categorized as the "ideal strength".

2.3 Zero-dimensional structure

This category includes nano-particles and clusters [48,49] as the solid structure and fullerenes [50-53] as the hollow one. While these do not maintain periodicity, they do possess characteristically beautiful, defect-free structure. Moreover, they are essential members of the family of nano-



(a) Structure of carbon nano-tubes, (9,0), (8,8), (8,2), and their unit cells.



(b) Relationship between the stress and the strain in the axial tension.

(c) Unbalanced load imposed on nano-tube.

Figure 6: Strength of carbon nano-tube[46].

structured materials. Thus, they should also be categorized into the "ideal structures".

In this section, the tensile behavior of the silicon cluster illustrated in Fig.7 (a) [26], which includes six atoms, is examined by the first-principle simulation (GGA, plane-wave basis set, and ultrasoft pseudopotential) as an example. The displacement is applied to the top and bottom of the cluster. Figure 7 (b) depicts the stretched process that discloses the spring-like behavior, and the load-displacement curve is shown in Fig. 7(c).

3 Ideal strength and instability

As described in the Introduction, the strength of an atomic structure is defined as the stress or strain at which unstable deformation takes place. Consequently, it is inevitable to investigate the instability criterion under an external load (or displacement) when we consider in detail the strength of nano-structured components.

3.1 Instability of homogeneous crystals under homogeneous external stress (strain)

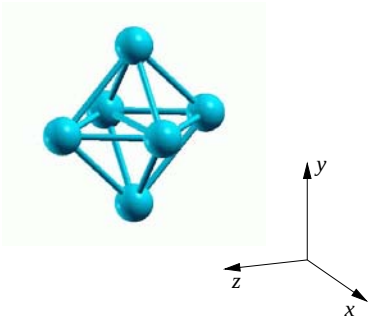
In the 1960s, Milstain [54] made a famous landmark analysis on the stability of cubic lattices under tensile deformation. The homogeneous deformation of cubic lattices is attributed to the components of the strain tensor in order that the distorted lattice shape is represented by the axial lengths, $a_1 - a_3$, and the angles, $a_4 - a_6$, as illustrated in Fig.8, respectively. It is then defined as "stable" when the total energy (free energy) of the system, Π does not decrease for an arbitrary incremental disturbance of strain under the external load. If it decreases, the component deforms without increase in external load, namely unstable deformation. Thus, the instability criterion for the homogeneous crystal under the homogeneous external strain is given by the sign of determinant A including its minor matrices. Here, the matrix A is in the form

$$\mathbf{A} = \left(\mathrm{A}_{ij}\right) = \left(\frac{\partial^2 \Pi}{\partial a_i \partial a_j}\right). \tag{1}$$

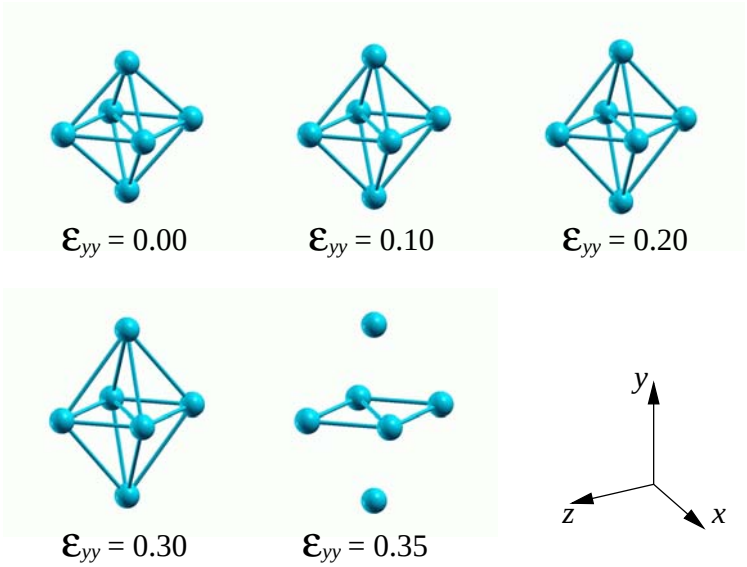
The lattice is stable when all of the determinants are positive. The criterion, of course, can be described by the differentials for strain instead of the variables a_1 to a_6. Since the elastic coefficient is defined as the second differential of the potential energy for the strain component, the instability criterion means the instance that the distorted structure loses its stiffness. Then, by using the elastic coefficient, the criterion for metals with cubic lattice (fcc and bcc) is rewritten as [1]

$$\begin{aligned} E_{xxxx} + 2E_{xxyy} &> 0 \\ E_{xyxy} &> 0 \\ E_{xxxx} - E_{xxyy} &> 0. \end{aligned} \tag{2}$$

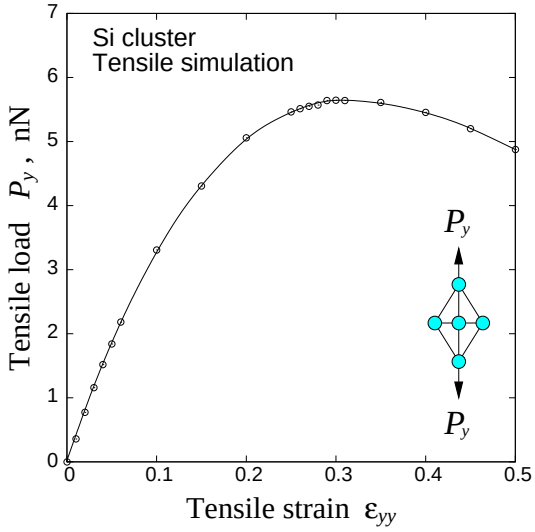
Hill [55, 56] pointed out that the instability criterion is dependent on the coordinates used for the evaluation of strain and stress. In other words, it is strongly dependent upon the loading boundary condition (loading device or external atomic system that yields the load on the



(a) Ideal structure of cluster consisted of six silicon atoms.



(b) Sketches of cluster in the elongated process.



(c) Relationship between the load and the strain under tension.

Figure 7: Strength of silicon cluster[26].

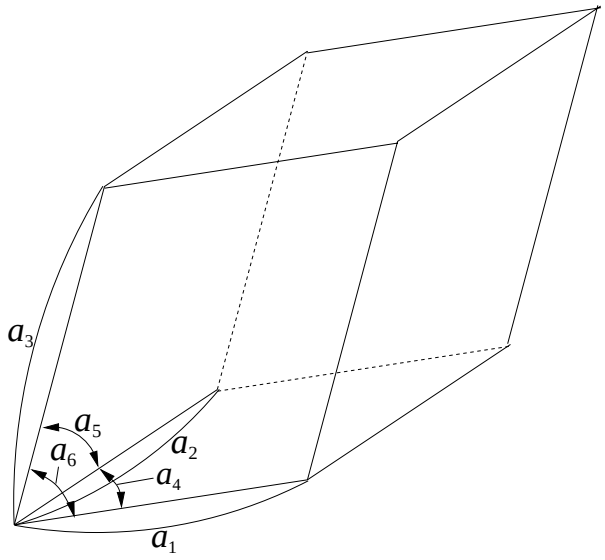


Figure 8: Variables $a_1 - a_6$ that represent the deformation of unit cell.

component in question). This stems from the fact that the freedom of deformation is restricted by only six variables in the analysis. As the nano-material has a larger number of degrees of freedom in general, the effect must be considered in discussions of the instability criterion.

Wang *et al.* [57,58] expanded the discussion on the basis of free energy and corrected the criterion using the stiffness coefficient for the bulk crystal. On the other hand, the criterion can be discussed in the context of the propagation of sound waves. The criterion of the transformation of crystal structures has been explored in terms of the soft mode of phonons by Hill [59]. As the elastic coefficient has a close relation with the long-wave mode of phonons, the ideal strength, which is a kind of structural transformation under an external load, surely can be generalized by the viewpoint of the soft mode, including the influence of the internal displacements. This phonon-based analysis is effective as far as the components hold periodicity, though the effect of external force is not explicitly included in the strictest sense.

Rapid progress in computational technology makes it possible for us to analyze the ideal strength on the basis of quantum mechanics. Investigations are rigorously conducted not only for pure metals with simple structures but also complex crystalline structures, *e.g.* intermetallic compounds. Sob *et al.* [60] produced an excellent review on the ideal strength of metals in the Highlight No. 58. In that report, they pointed out the importance on the coupling of ideal deformation (mechanical property) with electrical or magnetic properties in an ideal crystal. Several researchers (*e.g.* [60]) have successfully extended the analysis on the change in the electrical or magnetic properties due to deformation. For example, the electric property of the CNT is strongly correlated not only to its chirality but also to the strained condition [44-47].

3.2 Local instability in atomic components

In order to generalize the discussion on the "strength" of nano-structured components, it is necessary to explore the instability criterion of an arbitrary structure in the atomic scale.

The criterion for the dislocation emission from a crack tip under an external stress was proposed by Rice [61]. This have an impact on the following works on local instability of atomic components, though his analysis was totally based on the continuum mechanics concept. In his analysis, Rice derived the criterion from an instability of plastic flow under a singular stress-strain field near the crack tip, with the consideration given to the crystallographic slip direction. This stimulated researchers who were working on material strength at the atomic scale, leading to studies using numerical simulations by classical molecular dynamics (*e.g.* [62]). As a result, criterion based on the atomic mechanics concept is required to discuss the above problem precisely. In the nano-structured components, the switching or breaking of bonds between atoms under an external load generally brings about a sudden load-drop or displacement acceleration, namely unstable deformation. In a crystal, the dislocation nucleation was the shear collapse of local lattice. Thus, it was investigated from perspective of lattice instability [63, 64].

The stress, σ_{ij}, and the elastic coefficient, E_{ijkl}, are the quantities in continuum mechanics originally defined for a large region, which includes enough atoms. Those inherently can not be evaluated for each atom or local region. However, under the appropriate assumption (for example: the inter-atomic potential of embedded atom method [65]), σ_{ij} and E_{ijkl} in a local region can be reasonably estimated in consideration of short-range influence [66]. Vliet *et al.*[67] proposed the local instability criterion (Λ-criterion) based on the soft mode of long-wave phonons referring to the relationship between the long-wave property and σ_{ij} and E_{ijkl} in the region. They successfully applied it to dislocation generation under nano-indentation. Moreover, the criterion is generalized to the soft mode of shorter-waves by Dmitriev *et al.* [68].As we will describe in the next section, the exact mechanical criterion for the instability of arbitrary atomic structures under external load requires enormous numerical calculations due to its large number of degrees of freedom for deformation. Thus, it becomes important to make an approximation (local instability criterion) to extract the effective condition based on local information.

Strictly speaking, the analysis of phonons can be applied only on the structure with periodicity. As the low-dimensional structures discussed in section 2 do hold the periodicity in their dimensions, the characteristic instability can be explained by their soft mode. The instability at the surface of a nano-film with strained lattices has recently analyzed using the phonon dispersion property. The results may provide an important clue not only on the dislocation generation from the surface under strain, but also on the ideal strength of low-dimensional components.

3.3 Instability criterion for arbitrary structures under external load [69, 70]

Let us consider an arbitrary body comprising N atoms (N: number of atoms) under a strained state at the temperature of 0 K. Under an external load, the deformation is described by the number of degrees of freedom, $M = 3N - 6$, excluding the translation and rotation of the body. The total energy in the structure under an arbitrary deformation, Π which is the sum of strain energy, U, and the external work (negative), V, is in the function of only coordinates of atoms, $R = (R_1, \cdots, R_M)$. Then, the Taylor's series expansion of Π in terms of infinitesimal deformation, ΔR, gives the following relation

$$\Pi(\boldsymbol{R} + \Delta\boldsymbol{R}) = \Pi(\boldsymbol{R}) + \sum_{m=1}^{M} \frac{\partial \Pi}{\partial R_m} \Delta R_m + \frac{1}{2} \sum_{m=1}^{M} \sum_{n=1}^{M} \frac{\partial^2 \Pi}{\partial R_m \partial R_n} \Delta R_m \Delta R_n + \cdots . \quad (3)$$

The second term on the right-hand side vanishes since the system is at equilibrium. Attention should be paid on the fact that this term does not denote the external load.

Ignoring the higher-order terms, we have

$$\Delta\Pi \;=\; \Pi(\boldsymbol{R}+\Delta\boldsymbol{R}) - \Pi(\boldsymbol{R}) = \frac{1}{2}\,{}^t\Delta\boldsymbol{R}\,\boldsymbol{A}\,\Delta\boldsymbol{R}, \tag{4}$$

where the components of the matrix, A, are given by

$$A_{mn} = \frac{\partial^2\Pi}{\partial R_m \partial R_n}. \tag{5}$$

The structure is stable when $\Delta\Pi$ is positive, but becomes unstable and consequently deformation progresses when $\Delta\Pi$ becomes negative. Thus, the critical magnitude for the structural stability is given by $\Delta\Pi$ =0.

The matrix, A, is diagonalized using the matrix, P=(p_1 p_2 $\cdots$ p_M), where p_1, p_2,$\cdots$, p_M are the eigenvectors of A, as

$$\boldsymbol{P}^{-1}\boldsymbol{A}\boldsymbol{P} \;=\; {}^t\boldsymbol{P}\boldsymbol{A}\boldsymbol{P} = \begin{pmatrix} \eta_1 & & \boldsymbol{O} \\ & \ddots & \\ \boldsymbol{O} & & \eta_M \end{pmatrix}. \tag{6}$$

Here, η_m ($\eta_1 < \cdots < \eta_M$) is the eigenvalue of A. Introducing the matrix, $\Delta\mathrm{Q} = \mathrm{P}^{-1}\Delta\mathrm{R}$, we get

$$\begin{aligned} \Delta\Pi \;&=\; \frac{1}{2}\,{}^t\left(\boldsymbol{P}\,\Delta\boldsymbol{Q}\right)\boldsymbol{A}\left(\boldsymbol{P}\,\Delta\boldsymbol{Q}\right) \\ &=\; \frac{1}{2}\,{}^t\Delta\boldsymbol{Q}({}^t\boldsymbol{P}\boldsymbol{A}\boldsymbol{P})\Delta\boldsymbol{Q} = \frac{1}{2}\sum_{m=1}^{M}\eta_m\left(\Delta Q_m\right)^2. \end{aligned} \tag{7}$$

Then, the instability criterion ($\Delta\Pi$ =0) is attained by

$$\eta_1 = 0, \tag{8}$$

under

$$\Delta Q_m \;=\; 0 \quad (m = 2,\cdots,M). \tag{9}$$

(Strictly speaking, the third differential term in Eq.(3) must be negative.) Moreover, Eqs.(7)-(9) point out that

$$\Delta\boldsymbol{R} \;=\; \Delta Q_1 \cdot \boldsymbol{p}_1. \tag{10}$$

This means that the deformation at the instability is proportional to the eigenvector for the minimum eigenvalue, signifying the deformation mode at the instability. As the scheme is purely dependent on the system's energy, it can be applied to the quantum mechanical analysis without any collection.

Since the criterion is versatile, it is applicable to the instability of materials without periodicity or symmetry, such as the nucleation of dislocations [70], the delamination of thin film from a substrate [71], and so on. Even the plastic deformation of amorphous and metal glass, which stems the bond switching of local atoms, can be analyzed.

3.4 Structural instability

Above, we mainly discussed the instability of a lattice. In the meantime, there is another type of instability caused by the combination of load and global structures. It happens even when the lattice strain is not large. We can classify it into the "global" instability instead of "local" instability because it takes place in a macroscopic elastic body. A typical example of global instability is "buckling" of thin bar.

Figure 9 (a) [26] shows a silicon nano-wire with the same structure as the one shown in Fig.5(a). Axial compression is applied to the wire, of which calculation cell consists of 1 unit cube (Simulation A) or 5 cubes (Simulation B). The periodic boundary condition in the first-principle simulation (GGA, plane-wave basis set, and ultrasoft pseudopotential) fixes both ends of the wire. Simulation A, of course, exhibits extremely high strength, whereas the load-strain curve in Simulation B shown in Fig.9 (b) has low strength due to the buckling. This signifies that the buckling strength can not be predicted by the ideal strength, nor can it be explained in terms of local strain (local lattice instability). On the other hand, an analogy does exist for the relation between the nano-structured component and macroscopic continuum body. In this sense, the conventional continuum mechanics of an elastic body provides an interesting insight to the global collapse of nano-structured components such as devices and MEMS/NEMS. Moreover, it should be noted that the instability criterion discussed in section 3.3 can be applied not only to the local instability, but also to the global one.

4 Conclusion

We discussed the strength of nano-components with the ideal structure, with particular attention focused on the peak stress of low-dimensional material to extend the concept of the conventional ideal (theoretical) strength of a perfect crystal. In the same framework, we could discuss the ideal strength of grain boundaries and interfaces with periodicity, even though they are not nano-components. Materials possessing a super lattice structure, of course, should be such interesting targets. Thus, the "ideal structure" could be defined as the model structure by which simulation provides us with fundamental knowledge.

In the latter half of this paper, we investigated the instability that is closely related to the strength on nano-structured components. Since there are many unknowns in the instability criterion, further research is required.

In this review, we make no mention of not only the influences of temperature and chemical factors, but also of the deformation in the post-unstable criterion, the multiple instabilities (*e.g.* yielding in crystals) and irreversible cyclic deformation (*e.g.* fatigue). It is clear from the history of the strength of macroscopic components that these factors play also crucial roles in the strength of nano-structured components.

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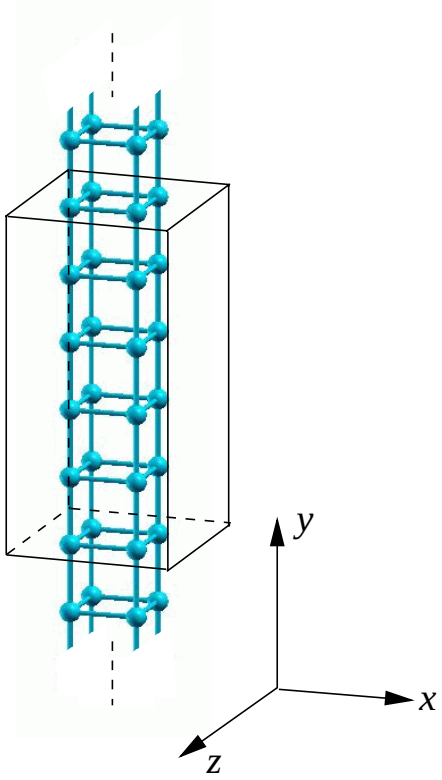
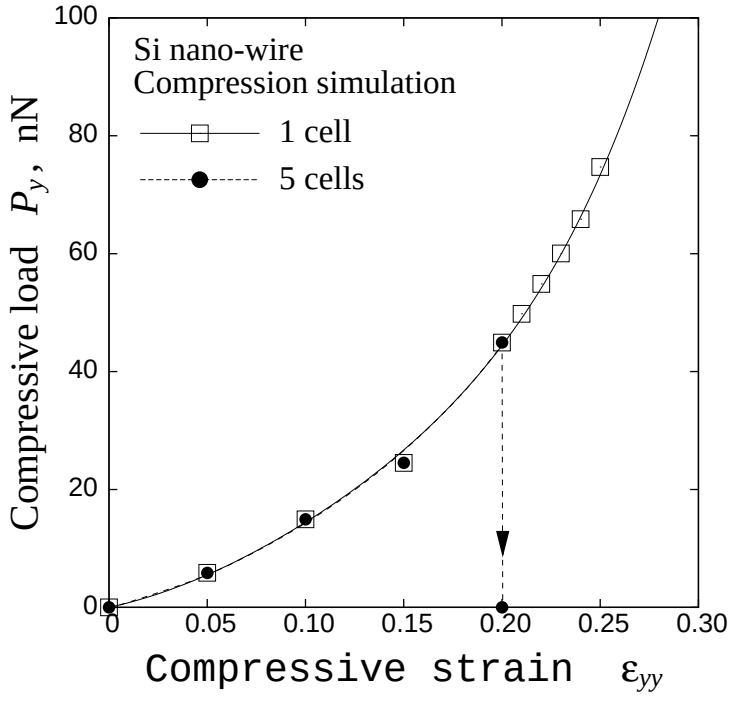


(a) Structure of nano-wire (5 cubes) for analysis of buckling.



(b) Relationships between the compressive load and strain. The sharp load drop in the wire with 5 unit cells point out the occurrence of buckling.

Figure 9: Buckling of silicon nano-wire as an example of global instability[26].

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