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Ideal Strength of Nano-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 structures, namely ideal structure. 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.

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. 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 (*e.g.* [5,6]).

(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 [6,7], signifying that the structure has a strong influence on 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 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 characteristic of 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.

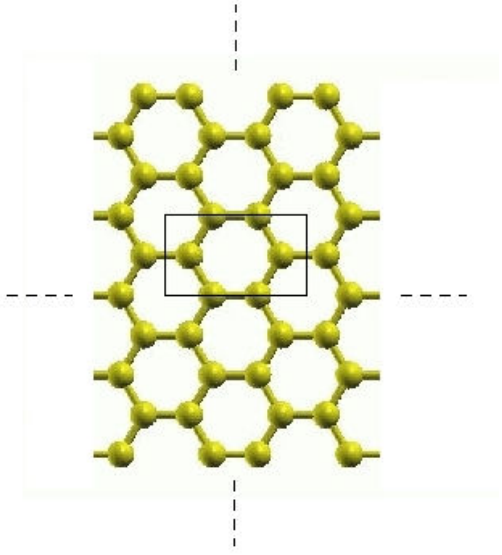
In the context of structural analysis, over last decade multi-scale simulation is spotlighted as an *ad hoc* method connecting molecular dynamics to continuum mechanics. However, it is necessary to identify the representative indicator for characterizing the strength of nano-structured materials as fundamental 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)).

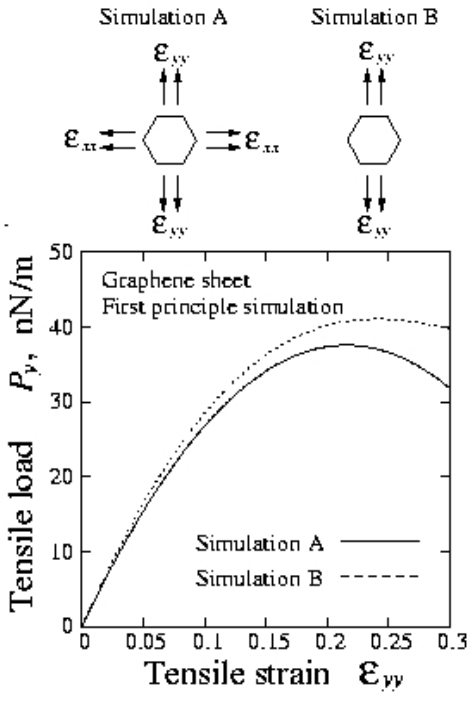
STRENGTH OF MATERIAL WITH IDEAL STRUCTURE

To analyze an "ideal" bulk crystal, the three-dimensional periodic boundary condition was applied to the unit cell [8,9]. 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.

Two-dimensional structure. 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 [10-14] which consists of a hexagonal carbon network as illustrated in Fig.1 (a). It is an absolute mono-layer film, for which the unit cell is indicated by the solid square in Fig.1 (a). 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 [10]. The dotted and solid lines in Fig.1 (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 psudo-potential). 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).



(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 1 Strength of graphene sheet

By comparing the load-strain curves, we can examine the validity of classical potential (*e.g.* the Brener potential [15]) and the tight-binding (TB) method [16] under the high-strain condition. The result obtained by TB showed excellent correspondence with that in the above first-principle analysis, whereas the Brener potential does not [10].

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 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. Since the thin film is interpreted as being a material sandwiched by the surfaces, the mechanical property reflects the nature of the surfaces. We may be able to determine the ideal surface effect on the strength by comparing the strengths between the bulk and the film [17,18].

For example, our analysis [10] on the strength of a silicon thin film with the excellent reconstructed surface of (100), of which the simplest structure is 1x2 by the first-principle simulation (GGA, plane-wave basis, ultrasoft pseudopotential) revealed that the peak stress increased as the film thickened, and approached the ideal bulk strength (thick line). It also revealed softening in the thinner film, signifying that the surface inherently possessed a weakening effect.

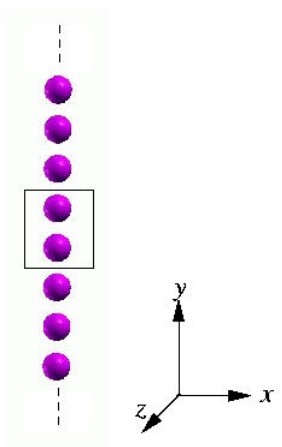
One-dimensional structure. There are several types of ideal wire with perfect one-dimensional periodicity, such as atomic chains, solid wires and tubes (hollow ones). In this section, we will present a typical strength analysis of them.

Atomic chain and nano-wire. 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.* [19]). Figure 2(a) illustrates the atomic chain in which atoms align in a string [20-23].

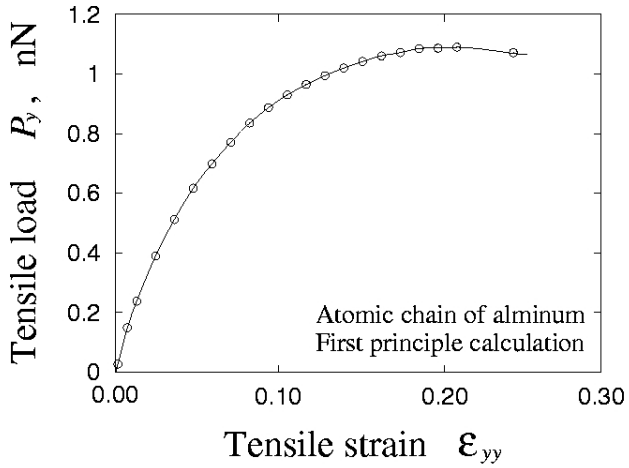
Numerical simulation (LDA, plane-wave basis set, and norm-conserving pseudopotential) is conducted on the calculation cell of an aluminum atomic chain shown by the square in Fig.2 (a) [22]. The result reveals that the equilibrium interval of atoms is much shorter than the closest distance between atoms in the bulk fcc crystal of aluminum. A tensile strain is then imposed on the cell. The load-strain curve shown in Fig.2 (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.2 (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 [22]. Therefore, we notice that the chain is more brittle than the bulk crystal.

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 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 still holds its periodicity along the wire axis, it should be categorized as an ideal wire as well. Figure 3 shows an example of the nano-wire structure proposed for silicon [18]. 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

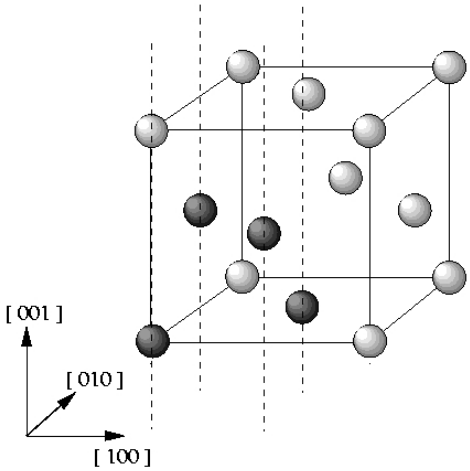
Tube. Since the discovery of fullerene, intensive research attention has been directed foward materials with hollow structures at the nano scale. As a wire, the carbon nano-tube (CNT) possesses beautiful tubular structure with rich properties, that have been rigorously investigated both experimentally and theoretically (e.g. [24-31]), promising potential use in future miniature devices and machines.



(a) Atomic chain.



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



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

Figure 2 Strength of aluminum atomic chain.

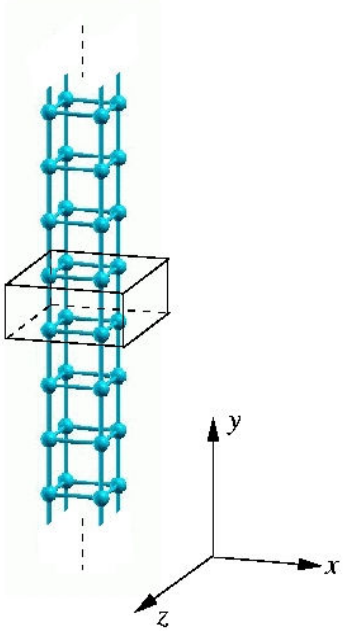


Fig. 3 Ideal structure of silicon nano-wire and the unit cell.

Figure 4 (left) 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 [30]. Here, (9,0) and (8,8) are known as Zigzag and Armchair types, respectively. Referring the graphene layer shown in Fig.1 (a), the strength of CNT (8,8) can be compared with that of raw material. (In the case of Fig.1 (b), the transverse strain is constrainted. For exact comparison, the simulation of the graphen 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.4 (right) 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, 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."

Zero-dimensional structure. This category includes nano-particles and clusters [32,33] as the solid structure and fullerenes [34-37] 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-structured materials. Thus, they should also be categorized into the "ideal structures."

The tensile behavior of the silicon cluster illustrated in Fig.5, 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. It shows the spring-like behavior under loading, and the load-displacement curve is shown in the figure.

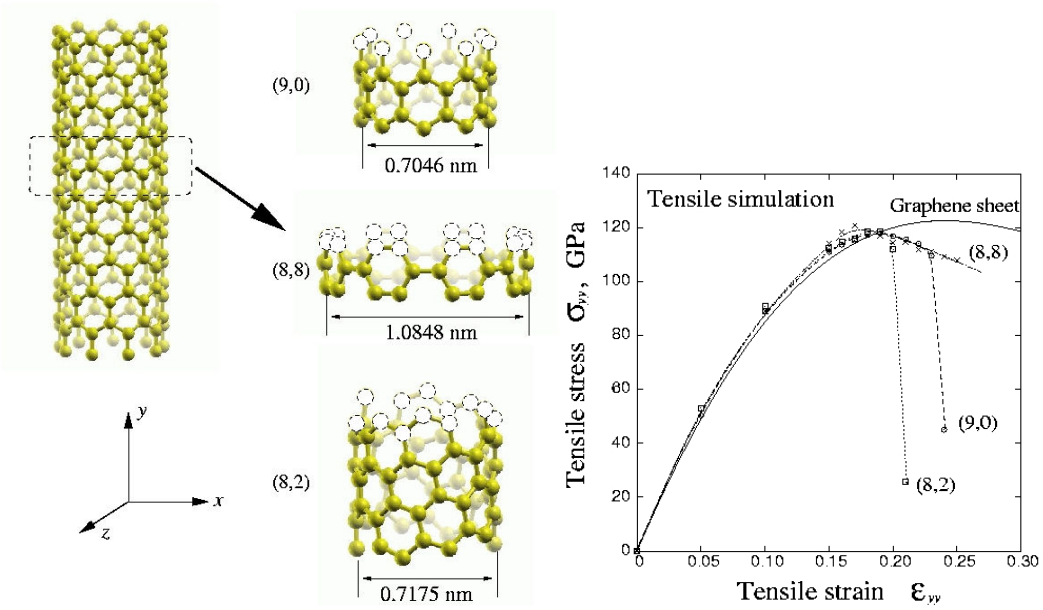


Figure 4 Strength of carbon nano-tube .

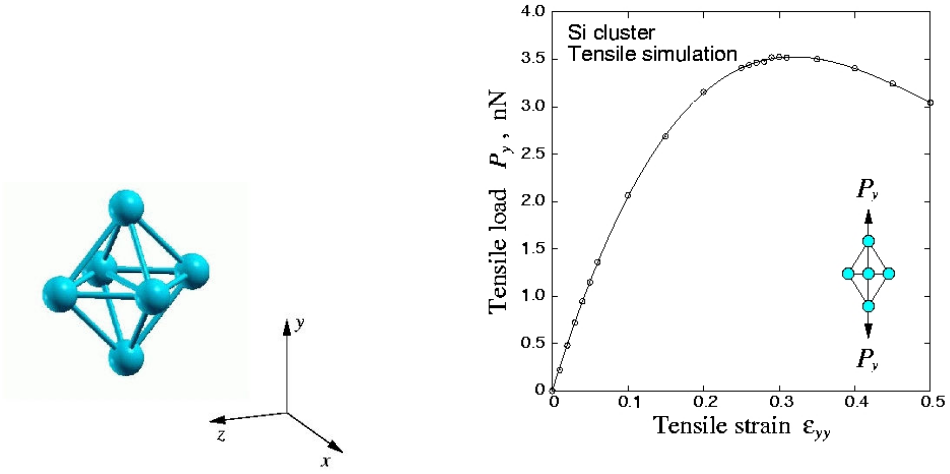


Figure 5 Strength of silicon cluster.

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 this article, 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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