

Ideal strength of diamond, Si, and Ge

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We have calculated the ideal shear strength and ideal tensile strength of C, Si, and Ge in the diamond structure. We find ideal shear strengths of 95 GPa, 6.5 GPa, and 4.5 GPa, and ideal tensile strengths of 95 GPa, 23 GPa, and 14 GPa for C, Si and Ge respectively. The shear calculation is performed on the $\{111\}$ slip plane sheared in a $\langle 112 \rangle$ direction, and the tensile load is applied in the $\langle 111 \rangle$ direction. We allowed for a full relaxation of the strains orthogonal to the applied strain as well as the atomic basis vectors.

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The mechanical properties of group-IV materials are of particular interest, as diamond is the hardest material known, while silicon and germanium are among the best understood materials, both experimentally and theoretically, due to their technological importance. One fundamental measure of the mechanical strength of a material is its ideal strength. The ideal strength is the stress required to deform a perfect crystal, and forms an upper limit to the strength of a real crystal. Stresses approaching the ideal tensile strength may occur near crack tips, and stresses approaching the ideal shear strength can be observed in nanoindentation studies. Nanoindentation experiments on diamond have shown that diamond can be converted into a graphitic structure by a shear stress,¹ while nanoindentation of silicon causes phase transformations underneath the indenter tip.²⁻⁷ Recently, calculations of the ideal tensile strength of diamond with the stress applied in the $\langle 111 \rangle$, $\langle 110 \rangle$, and $\langle 001 \rangle$ directions have been used to explain its preference for cleavage on the $\langle 111 \rangle$ plane.⁸ Calculations of the ideal shear strength of diamond have been used to explain the formation of graphitic structures during nanoindentation.⁹

In this paper we present the result of a comparative study of both the ideal tensile and shear strengths of diamond, silicon, and germanium (see Table I). The tensile strengths are calculated for a stress oriented in the $\langle 111 \rangle$ direction, which is expected to be the weak direction. The shear strengths are calculated for shear on the $\{111\}$ plane in a $\langle 112 \rangle$ direction.

The ideal strength is found by straining the crystal in a series of incremental strains, and simultaneously relaxing both the strain components orthogonal to the applied strain and the atomic basis vectors at each point. Because the calculation involves a strain applied to a perfect crystal, the calculation can be performed using a two-atom unit cell. The starting position for each strain step is taken from the relaxed coordinates of the previous strain step. This is necessary to ensure that the strain path is continuous.

The maximum in the stress, which occurs at the instability point, is the ideal strength. The stress is calculated both directly, from the Hellmann-Feynman theorem,¹⁰ and by taking a derivative of the energy with respect to the true strain, as described in Ref. 11. The total energy is computed as a function of strain using the pseudopotential total-energy scheme with a plane-wave basis set¹²⁻¹⁵ and density functional

theory in the local-density approximation. The pseudopotential is generated including semirelativistic corrections in the case of germanium,¹⁶ while the silicon and carbon pseudopotentials were generated without such corrections. A cutoff energy of 60 Ry was necessary for C, while a cutoff of 40 was sufficient for Si and Ge.

Figure 1 displays the stress as a function of shear strain for C, Si, and Ge, respectively. The filled circles correspond to the stresses calculated from the Hellmann-Feynman theorem, while the curve corresponds to the stress calculated from a derivative of a fit to the energy. In the case of diamond, the energy was only fit to the points before the instability because the energy changes abruptly after the instability point. Figure 2 displays the same data for the case of a tensile stress.

The properties of diamond under strain are dominated by the stability of its graphitic structure. Under either shear or tensile loads, shortly after instability, the structure was found to relax into a graphitic structure. This can be seen most clearly in Fig. 3, which shows the change in volume as a function of shear strain for the three systems. For the case of diamond, there is a jump in volume of 50% immediately after the instability point at 30% shear strain, corresponding to the difference in density between graphite and diamond. A similar transformation occurs under tension, which results in a positive pressure, because in this case the tensile strain is held fixed, which keeps the graphitic layers from separating freely.

In reality, broken diamond will not turn into graphite. However, this observation does correspond to the physical property of diamond which is its ability to form π bonds, and this effect will dominate the plastic and cleavage properties of this material. Specifically, carbon can exist in a favorable threefold coordinated structure, which forms when-

TABLE I. Ideal shear and tensile strengths.

	Shear load		Tensile load	
	Ideal strength (GPa)	Critical strain	Ideal strength (GPa)	Critical strain
C	93	0.3	95	0.13
Si	6.8	0.3	22	0.17
Ge	4.3	0.25	14	0.2

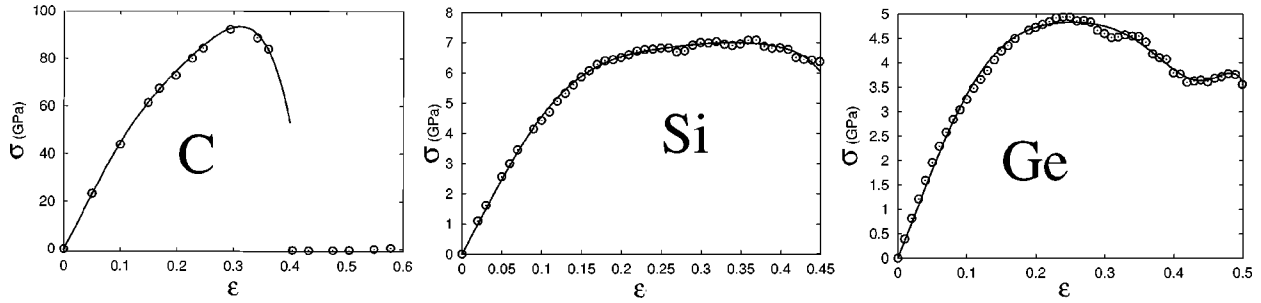


FIG. 1. Stress vs strain under shear load.

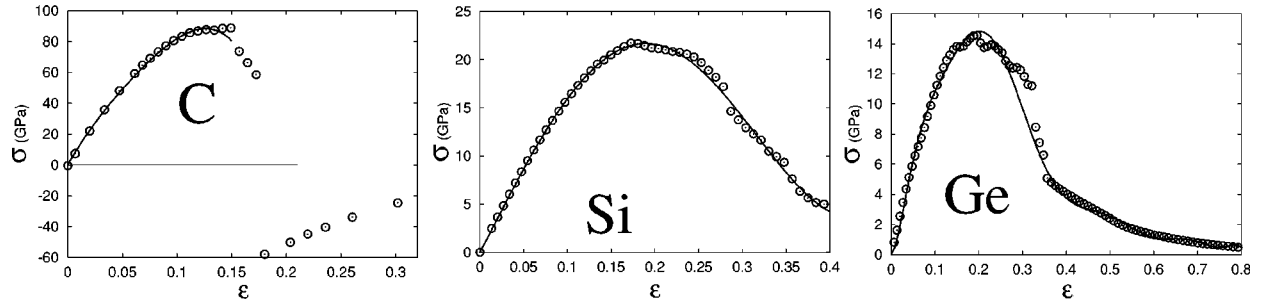


FIG. 2. Stress vs strain under tensile load.

ever bonds are broken in diamond. This affects vacancies, dislocation properties, and cleavage properties. The π -bonded chain surface reconstruction of the diamond (111) surface¹⁸ is an example of this.

Silicon and germanium display qualitatively similar behavior to one another, which is markedly different from that of diamond. These elements are unable to form strong π bonds because they have p electrons in their core. For this reason they do not prefer the graphite structure, which makes their instability much less dramatic than in the case of diamond.

Silicon and germanium both display a much lower tensile strength relative to shear strength that is seen in diamond. This can be explained to a certain extent by differences in the elastic constants of these materials. The Young's modulus of diamond in the $\langle 111 \rangle$ direction is 2.3 times its shear modulus, while the Young's moduli of silicon and germanium are both 4.2 times greater than their shear moduli. One surprising result of these calculations is that the ideal shear strength of silicon and germanium are both well below half of their ideal tensile strengths. A simple model of ductility would suggest that a material is ductile when its shear strength is less than half its tensile strength, since in that case dislocations would be expected to form and blunt a crack tip. In reality the picture is not nearly so simple. The stress field at a crack tip is actually closer to biaxial tension than uniaxial tension, and it is also highly inhomogeneous. Both of these effects can be expected to lower the stress required to open a crack, which could explain why these materials are brittle.

Another unusual feature of the low ideal shear strengths of silicon and germanium is that they are actually lower than the estimated Peierls stress. Using a simple Peierls-Nabarro model,¹⁷ one can obtain an estimated Peierls stress of 7 GPa

for silicon and 6 GPa for germanium, in each case higher than the calculated ideal shear strength. This suggests that at low temperatures dislocations in these materials may not be mobile, meaning that the entire lattice will become unstable before a dislocation can be induced to move. This could explain the observation of phase transformations underneath the indenter tip in nanoindentation studies of silicon,²⁻⁷ because the a lattice instability may actually precede dislocation mobility at low temperatures.

In conclusion, we have calculated the ideal shear and tensile strengths of diamond, silicon, and germanium. In dia-

Volume Changes Under Shear

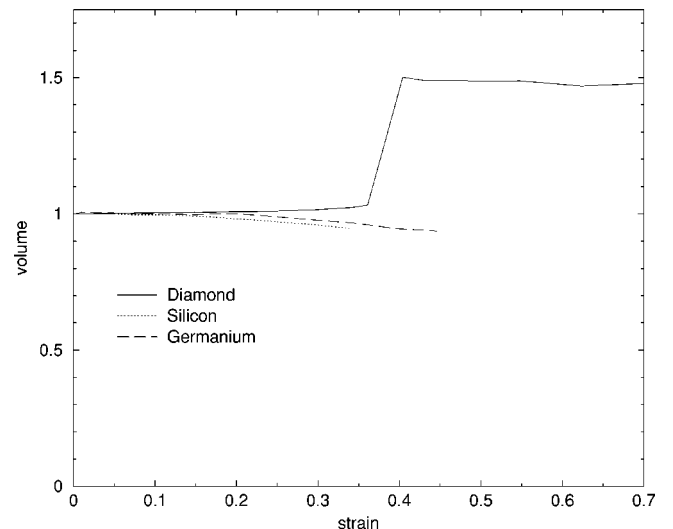


FIG. 3. Volumes vs shear strain for the three systems.

mond our calculations suggest a sudden transformation will occur at the critical stress to a graphitic structure under both shear and tensile stress. In silicon and germanium we see the surprising result that the ideal shear strength is significantly lower than the ideal tensile strength.

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