Two-Level Systems in the Mechanical Properties of Silicon at Low Temperatures

Recently, Kleiman, Agnolet, and Bishop (hereafter KAB) discovered some unexpected changes in the elastic properties of silicon at temperatures below 20 mK.[1] They offered a plausible explanation of their observations in terms of two-level defects similar to those that have become well known in glasses. They estimated that the number of defects required to account for their observations was 5×10^{16} cm^{-3}, about 1% of the concentration that produces similar effects in amorphous SiO$_2$. In view of the facts that the experiments used silicon crystals of high perfection and that silicon is probably the best known and thoroughly characterized material known, this result is surprising and invites a search for alternate explanations. I propose that the effects discovered by KAB could be produced by a relatively small concentration of electronic defects.

Indeed, a variety of electronic effects are known to produce low-temperature elastic softening over a wide range of doping concentrations.[2-5]

For the present case, consider a trapping defect with two states separated by a small energy difference. Only one of the states can be occupied because they occupy almost the same region of space. Acceptor impurities in silicon offer an example; small random strains cause small splittings of the acceptor ground states.[6,7] As strain from an acoustic wave changes the relative energies of the states, the populations of the levels change to minimize their free energy, and some of the strain energy is recovered. The time needed for level-to-level transitions to occur produces a frequency dependence and dissipation.

Let the energy levels of a center as a result of the random strain be $\pm V$ and the energy levels when a strain ϵ is applied be $\pm W = \pm(V + D\epsilon)$. The free energy of a center is

$$F = -W - kT\ln[1+\exp(-2W/kT)]\,. \tag{1}$$

The contribution to an elastic constant is determined by the second derivative of F with respect to ϵ at $\epsilon=0$. Because of the randomness, V and D are random variables, distributed over some range of values. The result must be summed over all centers in the crystal. For simplicity, consider rectangular distributions, m centers per unit volume in $dV\,dD$ for $V<U$ and $-\Xi<D<\Xi$. Then the total number of centers per unit volume is $N=2m\Xi U$ and it is found that

$$\Delta c = -(N\Xi^2/3U)\tanh(U/kT)\,. \tag{2}$$

As the temperature is increased, the effect decreases, becoming small as T exceeds U/k. The temperature dependence of the effect measured by KAB suggests that U is of order 10^{-6} eV. Values of Ξ in silicon are in the range 1-10 eV. Taking $\Xi=3$ eV, a $\Delta c/c$ of 10^{-5} is produced by only 3×10^{12} cm^{-3} centers.

The electronic effects contain a source for the amplitude dependence of the change in elastic constant reported by KAB. Since the energy differences involved are around 10^{-6} eV, with deformation potential constants of 3 eV, strains of 3×10^{-7} already produce nonlinear effects. Applied strains larger than the random strains of magnitude 3×10^{-7} in the above example cause very nonlinear changes in the thermal distribution of the occupancy of the states. In the electronic effect arising from shallow donors, the dependence of energy on strain fails to be quadratic when $\Xi\epsilon > U$.[2,8]

I feel that attributing the effects discovered by KAB to at least 10^4 fewer defects is an attractive alternative to their proposal. The same types of effects are known to be electronic in another temperature regime. There are many possible sources for little-known defects at concentrations less than 10^{13} cm^{-3}. A variety of metallic impurities are present at concentrations in the 10^{12} to 10^{13} cm^{-3} range. Pairing of impurities and defects present at higher concentrations might also produce low concentrations of novel defects. Phillips has also suggested a mechanism that requires a low concentration of defects.[9]

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