Bok and Combescot Respond: In their Comment,[1] Ambegaokar and Biswas (AB) agree that the instability that we described in our paper[2] is present in silicon and other covalent semiconductors, but might be overtaken by something else at the melting point. In our Letter[2] we already said that "the electron-hole instability, leading to a first-order phase transition, can be the one observed in melting." Using the parameters of silicon at room temperature, we found T^* of order of 2000 K. For the estimation of T^*, we used a paper of Heine and Van Vechten[3] (HVV), who calculated the softening of the transverse acoustic branch due to the creation of electron-hole pairs, i.e., the breaking of covalent bonds. The essential merit of the calculation of HVV is that it gives the experimentally observed variation of the energy band gap of silicon with temperature.

AB recently published a calculation of the same effect[4] (softening of the phonon frequencies) which they claim is more exact than that of HVV. We think that to compare their calculation with well-known numbers in silicon, they should compute the free energy of the phonon system at low plasma density ($< 10^{19}$ cm^{-3}) and check their value with the measured variation of the band gap (chemical potential of electron-hole pairs) with temperature.

In their Comment,[1] AB estimate an instability temperature T^* by taking only a fraction r of the phonons to soften linearly with the electron-hole pair density n. By taking arbitrarily $r = 0.4$, they find $T^* = 5000$ K. But this procedure is incorrect in the framework of their own model. They find that all branches of phonons change their frequencies with increasing n. To compute correctly T^*, they should estimate the total free energy F_{ph} of the whole phonon system including the six

phonon branches. This should give a much more rapid reduction of F_{ph} and thus a much lower value than estimated by AB.

Finally, we wish to remind that the estimate of T^* needs parameters, which are known only at room temperature, and so we think that our conjecture cannot be rejected by a theoretical calculation of T^*, which might be valid only within a factor 2. However, as the intrinsic carrier density close to T^* is found to be of order 10^{21} cm^{-3} (i.e., 2 orders of magnitude larger than the usually quoted value of 2×10^{19} cm^{-3} for Si at melting), experimentalists are the ones who could reject this conjecture by measuring the electron-hole plasma density of a silicon sample in a furnace, just before melting.

It is also possible that silicon may change from a tetrahedrally bound solid to a metallic liquid (i.e., melt) at a temperature lower than the one leading to an inflection point in the free energy, by thermal excitation through the energy barrier, as for any nucleation process.

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[1]V. Ambegaokar and R. Biswas, preceding Comment [Phys. Rev. Lett. 50, 285 (1983)].
[2]M. Combescot and J. Bok, Phys. Rev. Lett. 48, 1413 (1982).
[3]V. Heine and J. A. Van Vechten, Phys. Rev. B 13, 1622 (1976).
[4]R. Biswas and V. Ambegaokar, Phys. Rev. B 26, 1980 (1982).

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