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LETTER

The nature of the transition from supercooled liquid metal Si to the disordered solid phase, with possible implications for B

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The melting of crystalline silicon is well known to result in a metallic liquid. But when this is supercooled, it leads to a 'glass' transition to a non-metallic solid. This prompts us to first propose that in this 'metastable' phase transition the driving mechanism is the Coulomb repulsion between the electrons, the atomic structure remaining largely intact across the transition. This proposal then leads us to draw attention to the likely interest of the now very complex bonding in crystalline boron. Again, as with the simple sp^3 bonding in Si, melting produces a metallic liquid in which supercooling is possible and for which earlier diffraction studies have proved possible using levitation techniques. It will be of interest to determine experimentally whether a glassy state exists for B, as single-component glasses are rare, only Si and S being known currently from diffraction experiments.

Keywords: liquid metals; glass transition; brittle-to-ductile transition

One of us has earlier been concerned with understanding the X-ray diffraction measurements on amorphous Si, using a quantum-chemical electron density distribution based on sp^3 hybridization [1]. It has also been known for some time that, on melting crystalline Si, one is led to a metallic liquid. Important use was made, fairly recently, of levitation techniques [2] to study the supercooling of this liquid phase of Si. It is relevant to note at this point that similar X-ray studies have been made on the metallic liquid created by melting crystalline B to which we shall return briefly below.

Next we wish to draw attention to recent work on chemical bonding in both crystalline silicon and graphite in which Klein and March [3] (see also [4]) have put forward a quantum-chemical interpretation of the brittle-to-ductile transition (BDT). While such a transition is well established in Si, it was emphasised in [3] that it should also occur in graphite. Since graphite has a melting temperature T_m of ~ 4600 K (Si has $T_m = 1688$ K), it has been suggested in [3] that the BDT in graphite should be looked for experimentally around 3000 K. This was because of the link known to materials scientists between the melting temperature T_m and the temperature T_{BDT} of the BDT, the latter, roughly speaking, being a fraction of the former. Therefore, one was led in [3] to view the BDT in Si as a precursor transition to melting and to the proposal that a similar qualitative picture ought to apply also to graphite.

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With the above said information as background, a major focus of this Letter will be on metastable phases of (i) silicon, already summarised above, and (ii) the complex chemically bonded material boron. Si- and B-condensed phases have the common property that their liquid forms are metallic but their crystalline phases are not. It is then quite clear that in both these materials the nature of the interatomic force fields must change crucially on melting.

Therefore, it is to be stressed that in [3] an alternative way of describing the quantum chemistry in deriving the BDT in Si (and perhaps also in graphite) is via topological defects. These defects in [3] were disclinations, and already as Hafner [5] summarises, Nelson *et al.* [6], but now mainly in two-component systems (see, in this context, [7]) has interpreted the structure factor $S(\mathbf{q})$ of supercooled liquids in such terms. This is especially important to know in materials like Si and B, where the changes in interatomic forces on melting make any force field approach to $S(\mathbf{q})$ too specialised to be generally useful. The consideration of Nelson *et al.* [6] also shows the relevance of Frank's proposal [8] of icosahedral clusters to explain the remarkable range of supercooling of simple liquid metals [9]. It is also significant that disclinations can be defined in amorphous phases, and this is partially valuable since a BDT is known to exist in such materials without long-range translational order [3].

Finally, returning to boron, with $T_m=2360$ K, we expect amorphous B, and a supercooled liquid phase at 2090 K [2], if found to exist, will be non-metallic, this 'metastable' transition then being driven, as for Si, from supercooled liquid metal to non-metallic, but now disordered, solid by long-range Coulomb interactions. But, of course, this proposal as to the existence of B glass is a matter for experiment to settle in the future. It is potentially of considerable interest, because Si and S [10] are the only known one-component glasses presently, from available experimental diffraction studies [1,10].

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