Network-modifying ions in glass

SIR — Vessal *et al.* claim[1] to have found evidence in a computer-simulated model for microsegregation of network-modifying ions in glasses and also for high coordinations (5–6) of non-bridging oxygens around the network-forming cations, and vice versa. However, a completely different interpretation can be placed on their simulation results.

Vessal *et al.* find that the positions of the peaks for M–Si correlations (where M is Na or Rb) correspond to bond angles subtended at the intervening oxygen atoms of θ (M–O–Si) ~ 100°; such small angles are taken to imply that the average coordination number of such O atoms is considerably larger than that characteristic of normal bridging oxygen sites (2). Further, the average coordination of all types of O in the simulated structure is ~3; since 60% of the O atoms are bridging, Vessal *et al.* therefore conclude that the coordination of the remaining non-bridging oxygens is ~5 (ions), and hence, the coordination of non-bridging oxygens around the M^+ ions is also ~5 by charge balance.

But these data are also consistent with there being, on average, about one non-bridging oxygen in the nearest-neighbour coordination shell of the M^+ ions. Let us assume that in fact there is only one nearest-neighbour non-bridging oxygen to an M^+ ion; all the other (4–5) oxygen atoms surrounding the ion are therefore bridging, each covalently bonded to two Si atoms. If the most probable Si–O–Si bond angle is taken to be ~ 155° (ref.1) and if it is assumed for simplicity that the M^+ ions lie at the bisector of the Si–O–Si bond angle (on the side away from the Si atoms) and that all four such Si, O and M atoms are coplanar, the average M–O–Si bond angle is then 102°, very close to that observed in the model. Further, if we assume that the total average oxygen coordination of the M^+ ions is 6 (five bridging oxygens and one non-bridging oxygen), because the effective coordination of each bridging oxygen is in fact 3 (2 Si and 1 M) and that of each non-bridging oxygen is 2 (1 Si and 1 M), the overall average oxygen coordination number is 2.83, again very close to that observed.

The first peak in the Na–O and Rb–O partial radial distribution functions (RDFs) in ref. 1 is markedly asymmetric, with a pronounced tail at high *r*. The peak maximum in both cases occurs at a distance corresponding to the sum of ionic radii for cation ($r(Na^+)$ = 0.97 Å, $r(Rb^+)$=1.47 Å) and doubly charged oxygen ($r(O^{2-})$=1.32 Å). However, it is significant that the mid-point of the high-*r* tails corresponds to distances involving singly-charged oxygen ions ($r(O^-)$=1.76 Å), that is *r*(Na–O)=2.73 Å and *r*(Rb–O)=3.2 Å. There is evidence[2] that partial charge transfer occurs in v-SiO_2, and thus we can associate O^- configurations with bridging sites, and O^{2-} configurations with non-bridging sites. Thus, analysis of the shape of the first peak in the alkali-oxygen partial RDF is also consistent with the present interpretation of a mixed first coordination shell containing both bridging and non-bridging oxygens. In our molecular dynamics simulation[2] of lithium silicate allowing for charge transfer, such a mixed Li-O coordination shell was found.

On the matter of cation microsegregation, Vessal *et al.* claim that the observation of first (O), second (M), third (O) and fourth (M) nearest neighbours around every alkali ion demonstrates clustering of the ions exceeding that which would be expected on the basis of an even distribution of the ions throughout the structure. The partial RDF for correlations between interstitial voids in a model of v-SiO_2 exhibits (broad) peaks at ~4 and ~8 Å, and so even in the simplest model for an alkali-modified silicate glass, in which the M^+ cations randomly occupy the interstices in the silicate framework, one would expect cation–cation correlations at distances comparable to those found experimentally and in the simulation.

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What is a chaperonin?

SIR — Ursic and Culbertson[1] assert that yeast and *Drosophila* TCP1 proteins lack two attributes generally shared by chaperonins (*sic*) in that they are neither members of multigene families nor heat-shock proteins. These authors have confused the terms 'chaperonin' and 'molecular chaperone'. 'Chaperonin' refers to ubiquitous, sequence-related proteins, including the Rubisco subunit-binding protein of plants and the GroE proteins of *Escherichia coli*. These chaperonins are a type of 'molecular chaperone', a protein required for the post-translational folding, targeting or assembly of other proteins but which does not itself form part of the final assembled structure.

Even allowing for a confusion between these two terms, however, neither of the attributes mentioned by Ursic and Culbertson are general characteristics of either chaperonins or molecular chaperones. Some, but certainly not all, molecular chaperones are heat-shock proteins. The *E. coli groE* operon is a good counterexample to the statement that chaperonins or chaperones are typically encoded in multigene families.

The report[2] to which Ursic and Culbertson referred proposed that TCP1 and TF55 may function as molecular chaperones. The question of possible evolutionary relatedness of TCP1 and chaperonin-60 genes was also raised in that report and it was concluded that no sequence similarity existed (see Table 1 of ref. 2). It is clear from inspection of TCP1 and chaperonin-60 amino-acid sequences, however, that similarities exist between these two proteins. These similarities are present in register throughout both types of sequences. The figure shows one region of similarity. The chaperonin-60 sequences presented were chosen to represent a wide range of phyla. These similarities are statistically highly significant according to the criteria of Schuler *et al.*[3]. These observations suggest a common origin for the *TCP1* and chaperonin-60 genes.

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                    *   +++** +  +  + +        ++   + *
Dm TCP1     ...DIGDVTVTNDGATILRLLEVEHP....AAKVLVELAQLQ     85
Cg TCP1     ...DIGDVTITNDGATILKLLEVEHP....AAKVLCELADLQ     82
Sc TCP1     ...DIGDFTVTNDGATILSLLDVQHP....AGKILVELAQQQ     90
Bn Cpn60β   ...KYGSPRIVNDGVTVAREVELEDPVENIGAKLVRQAAAKT     77
Bn Cpn60α   ...EFGSPKVVNDGVTIARAIELPDAMENAGAALIREVASKT     75
Ec Cpn60    ...SFGAPTITKDGVSVAREIELEDKFENMGAQMVKEVASKA     75
Hs Cpn60    ...SWGSPKVTKDGVTVAKSIDLKDKYKNIGAKLVQDVANNT     77

                     *****     *    +     +     *  +  *
Dm TCP1        DEEVGDGTTSVVILAAELLKNADELVKQKIHPTSIISGY... 124
Cg TCP1        DKEVGDGTTSVVIIAAELLKNADELVKQKIHPTSVISGY... 121
Sc TCP1        DREIGDGTTSVVIIASELLKRANELVKNKIHPTTIITGF... 129
Bn Cpn60β      NDLAGDGTTTSVVLAQGFIAEGVKVVAAGANPVLITRGI... 116
Bn Cpn60α      NDSAGDGTTTASVLAREIIKHGLLSVTSGANPVSLKRGI... 114
Ec Cpn60       NDAAGDGTTTATVLAQAIITEGLKAVAAGMNPMDLKRGI... 114
Hs Cpn60       NEEAGDGTTTATVLARSIAKEGFEKISKGANPVEIRRGV... 116
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Aligned TCP1 and chaperonin-60 amino-acid sequences (incomplete). The numbers refer to Dm (fruitfly), Cg (hamster), Sc (budding yeast), Bn (*Brassica napus*), Ec (*E. coli*), Hs (human). GenBank accession numbers are M21159, M34665, M21160, M35600, M35599, X07850 and M34664, respectively. The alignment was made using the MACAW program[3]. Asterisks, positions at which all seven sequences have the identical amino acid. Crosses, positions at which at least two TCP1 sequences and two chaperonin-60 sequences have the identical amino acid.

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