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COMPUTER MODELLING OF PLASTICITY IN MINERALS
- THE HYDROLYTIC WEAKENING OF QUARTZ

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In the two decades since the hydrolytic weakening effect in quartz was observed in the laboratory /1/, there has been a consistent effort, firstly, to identify the water-related weakening agent and, secondly, to establish whether this agent primarily affects dislocation mobility or dislocation density. The experimental situation is still uncertain and has been extensively reviewed elsewhere /2,3,4,5,6/, but by means of atomistic computer modelling we have obtained some evidence for the identity of the water-related species and for a mechanism by which it can increase dislocation mobility /7,8/.

Our method was first to find a potential function that could reasonably describe the elastic, phonon and internal strain properties of the perfect α -quartz structure /9,10/. This potential function was based on a covalent description of the SiO_2 network: the energy of Si and O atoms depending on Si-O and O-O lengths and Si-O-Si and O-Si-O angles. With the potential we could calculate the energy of distorted SiO_2 structures, providing there were no broken bonds. We could also estimate the relative energies of water and hydroxyl groups in different configurations in the SiO_2 network by regarding the hydrogen as merely saturating oxygen dangling bonds and arguing that the energy of each O-H bond should be more-or-less independent of its environment.

With this potential we found the structure of perfect dislocations in α -quartz with low energy cores /9,10/ and then looked at kink pair nucleation and migration on one of them. The dislocation had Burgers vector $\underline{a}_1$ and line direction $\underline{a}_2$ (referring to hexagonal lattice vectors) and was labelled B60a. The lowest energy structure for the core was labelled H3C4 and it had a core energy of 3.0 eV for a core radius of 7.4 Å. The kink nucleation energy was about 5 eV and it was independent of kink separation, within the accuracy of our determination. A rough estimate of the migration energy gave a minimum value of 4.2 eV. Very approximate values for these energies have been obtained experimentally from dislocation motion around crack tips in dry quartz /3/ - they are about 3 eV for nucleation and 6 eV for migration, comparable with our estimates.

In wet quartz the possibility had been suggested /11/ that water could act like a dopant in a semiconductor and that kink nucleation and migration energies would be lowered by charge transfer. However, we were unable to find a credible water-

related structure that could act in this fashion /8/. It turned out that the original hypothesis /1/ of $\equiv \text{Si-O-Si} \equiv$ being hydrolysed to $\equiv \text{Si-OH HO-Si} \equiv$ was more likely, reducing the kink pair nucleation energy to between 2 and 3 eV. The reason for this large drop was the release of strain in the kink pair caused by cutting a very stretched bond. More elaborate mechanisms for kink pair nucleation involving non-abrupt kinks and allowing the hydroxyl groups to separate led to a further lowering of the kink pair nucleation energy to less than 1 eV.

Similar results were also obtained for MacLaren's model of the water defect /12/, which can be thought of either as 2 H_2O molecules replacing one SiO_2 formula unit or 4 H atoms replacing one silicon atom, i.e. $(4\text{H})_{\text{Si}}$. Our conclusion was that both localised, hydrolysis models due to Griggs /1/ and to MacLaren et al /12/ could be responsible for hydrolytic weakening, through a profound increase in dislocation mobility.

Finally, it should be noted that our original calculations with the phenomenological potential function have been reinforced by ab-initio, local density functional calculations of $\equiv \text{Si-O-Si} \equiv$ hydrolysis and the subsequent interaction of hydroxyl groups /8/.

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