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Structure and stability of grain boundaries in doped fluorite crystals from atomistic simulation

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It is well known that dopant atoms in a material can segregate to grain boundaries (GBs), and that the corresponding changes in the structures of the GBs can affect key properties of the material such as its conductivity. There is hence considerable interest in using computer simulation to determine, for a given dopant element and concentration, the effect of segregation on GB structure and stability for different types of GB. We have used Monte-Carlo-based simulation methods to study GB segregation in doped fluorite oxide crystals. We have found that these methods enable atomic-scale GB structures to be calculated efficiently. Our simulations suggest an interesting richness of equilibrium GB structures in doped fluorite oxides. To elaborate, we characterised the structures of eight twin GBs in doped ceria for a wide range of dopant concentrations and temperatures, and observed a wide variety of structures. Moreover, for certain GBs we observed first-order complexion transitions at certain concentrations. We also quantified the effect of doping and segregation on the stability of the GBs, finding, for instance, that doping with Zr acts to stabilise GBs in ceria in general. The simulation methods we have employed could thus prove useful for studying GB segregation phenomena in similar systems. The figure here shows structures of the 210 twin GB obtained from our simulations at 1000K and various Zr concentrations up to the miscibility-gap concentration. Only cations are shown, and are given a size and colour which reflects the probability of the cation site being occupied by Zr or Ce.