Electronic Structure of β-SiAlON: Effect of Al/O Doping and of Finite Temperature

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Abstract. Electronic structure of a series of ordered and disordered β-$Si_{6-z}Al_zO_zN_{8-z}$ systems is investigated by means of ab initio calculations, using the FLAPW method as implemented in the wien2k code and Green function KKR method as implemented in the spr-kkr code. Finite temperature effects are included within the alloy analogy model. We found that the trends with the Al/O doping are similar for ordered and disordered structures. The electronic band gap decreases with increasing z by about 1 eV when going from z=0 to z=2. The optical gap decreases analogously as the electronic band gap. The changes in the density of states (DOS) at Si and N atoms introduced by doping β-Si_3N_4 with Al and O are comparable to the DOS at Al and O atoms themselves. The bottom of the conduction band in β-$Si_{6-z}Al_zO_zN_{8-z}$ is formed by extended states residing on all atomic types. Increasing the temperature leads to a shift of the bottom of the conduction band to lower energies. The amount of this shift increases with increasing doping z.