Model of grain boundary diffusion in titanium and zirconium α- and β-phases

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Titanium and zirconium are advanced construction materials widely used in nuclear industry and extensively applied in medicine. Both metals are characterized by abnormally low values of grain boundary diffusion activation energy Q_b in low-temperature α-phase. Expressed in dimensionless form Q_b/kT_m (k – Boltzmann constant, T_m – melting temperature), these values are 6 and 7 for titanium and zirconium respectively. These values are below respective energies typical of single-phase metals such as copper and aluminum (9 and 10 respectively), and grain boundary diffusion activation energy Q_b in high-temperature β- phase which is 9.5 kT_m for titanium and 10 kT_m for zirconium. Currently there is no model describing any reasons for abnormally low values of grain boundary diffusion activation energy in titanium and zirconium α-phase.

Paper [1] suggests a phenomenological theory of nonequilibrium grain boundaries (TNGB) which allows calculating Q_b values in pure metals which are lacking any structural transitions. Proceeding from this theory, the boundary consists of islets of 'amorphous' and 'solid' phases. The ratio of the volume fractions of these phases is proportionate to the free volume of the boundary. The process of grain boundary diffusion is triggered by fluctuations of structural amorphization or 'melting' during which 'corridors' appear in the boundary between islets of the 'amorphous' phase along which diffusion transfer occurs. Thus, the grain boundary diffusion activation energy appears to be related to the volume fraction of the amorphous phase islets and consequently to the free volume of grain boundaries. The theory carefully describes diffusion processes in single-phase materials, however, it is inapplicable to calculate parameters of grain boundary diffusion in titanium and zirconium, because these metals at elevated temperatures experience polymorphic transformation the thermodynamics of which affects the kinetics of heterophase amorphization fluctuations.

Based on generalization of TNGB approaches, the paper suggests a theory of grain boundary diffusion in metals undergoing phase transitions. Thermodynamic parameters of these fluctuations were calculated and self-consistent phenomenological models of boundary structures in α- and β-phases were suggested. Abnormally low values of the grain boundary diffusion activation energy in low-temperature titanium or zirconium α-phase are explained by contribution of additive components associated with the release of energy in phase transformations to the free energy of heterophase amorphization fluctuations. Values of the grain boundary diffusion activation energy in titanium and zirconium α- and β-phases that were obtained on the basis of the developed model with a high degree of accuracy conform to the experimental data.

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References

[1] V.N. Chuvil'deev *Non-equilibrium grain boundaries. Theory and applications*. Moscow: Fizmatlit. 2004. 304 p. (in Russian).