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Thermal expansion in isomorphic Me_5Si_3 (Me=transition metal) compounds

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Transition metal silicides have been investigated due to the applications in several fields, such as: structural materials, electronic devices, nuclear industry. The physical properties including mechanic, electric, magnetic, thermal, optical, etc. of these compounds are strongly dependent of the metallic atoms and their atomic bonds. The family of silicon-based compounds of Me_5Si_3 stoichiometry, known as Nowotny phases, where Me is a IV, V or IV transition metal element crystallize in three different structures: 1) Ti_5Si_3, Zr_5Si_3 and Hf_5Si_3 compounds crystallize in a hexagonal structure obeying P6/mcm symmetry and (Me: 4d and 6g, Si: 6g) Wyckoff positions; 2) Compounds such as V_5Si_3, Cr_5Si_3, Mo_5Si_3, W_5Si_3, βNb_5Si_3 and βTa_5Si_3 crystallize in so-called T_1 structure with I4/mcm space group and (Me: 4b and 16k, Si: 4a and 8h) Wyckoff positions and 3) Compounds such as αNb_5Si_3 and αTa_5Si_3 crystallize also in a tetragonal structure, called T_2, in same I4/mcm space group but different Wyckoff positions (Me: 4c and 16l, Si: 4a and 8h). The measurement of the thermal expansion coefficients of these compounds by high temperature X-ray diffraction shown that they are strongly dependent of the metallic atoms. Since these compounds crystallize in hexagonal or tetragonal symmetry, the thermal expansion is anistropic. The anisotropy of the thermal expansion in these materials have been controlled by the following ways: 1) by partial substitution of the metallic atom by another metallic atom to promote the formation of solid solutions, or 2) by formation of ternary compounds, by partial substitution of silicon by boron in the structures, for example. Since these compounds present high melting temperatures, they are prepared in polycristalline form by arc-melting process followed by heat-treatment at temperatures above 1400 K. The thermal expansion coefficients of Me_5Si_3 compounds have been analyzed taking into account the crystal structure of these compounds.

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