

# The Influence of $d^{10}$ - $d^{10}$ Interactions in $\text{Ag}_5\text{Te}_{1.8}\text{Se}_{0.2}\text{Cl}$ and $\text{Ag}_5\text{Te}_{1.6}\text{Se}_{0.4}\text{Cl}$ on Structural and Thermoelectric Properties

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Measurements of the thermopower and of the thermal diffusivity and a detailed analysis of the structural features by temperature-dependent single-crystal structure determinations of silver ion-conducting  $\text{Ag}_5\text{Te}_{1.8}\text{Se}_{0.2}\text{Cl}$  and  $\text{Ag}_5\text{Te}_{1.6}\text{Se}_{0.4}\text{Cl}$  were performed to investigate the interaction of silver ions in their disordered state. The substituted phases show an order/disorder phase transition at 273.3(2) and 302.5(2) K, respectively, accompanied by a drop of the thermal diffusivity and a minimum plateau of the thermopower right after the transition. Silver ions are arranged in well-defined strands along the crystallographic  $c$  axis characterized by a set of not fully occupied sites.  $\text{Ag}_5\text{Te}_{1.6}\text{Se}_{0.4}\text{Cl}$  shows a negative thermal expansion during temperature rise right after the silver order/disorder phase transition; this is explicable by attractive  $d^{10}$ - $d^{10}$  interactions within the disordered silver substructure. After the minimum values of the thermopower have been reached, these values rise in parallel to the decrease of the  $d^{10}$ - $d^{10}$  interactions.  $\text{Ag}_5\text{Te}_{1.6}\text{Se}_{0.4}\text{Cl}$  shows a very low value of the thermal diffusivity of  $0.070 \text{ mm}^2 \text{ s}^{-1}$  at 300.7 K.

*Key words:* Silver, Tellurium, Polytelluride, Thermoelectrics,  $d^{10}$ - $d^{10}$  Interactions