Thermoelectric power of $CuTa_2O_6$:Sb semiconductors

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The $CuTa_{2-x}Sb_xO_6$ solid solution is a semiconductor and the energy gap estimated by the Kubelka-Munk method decreased from 2.94 to 2.64 eV for $0.0 \leq x \leq 0.50$ with increasing degree of incorporation of Sb^{5+} ions replacing Ta^{5+} ions in the lattice of $CuTa_2O_6$ [1]. $CuTa_2O_6$ is a promising practical photocatalyst. The cubic phase of $CuTa_2O_6$ supported a higher methyl orange dye degradation efficiency than the orthorhombic phase [2].

Electrical conductivity σ(T) of the samples under study was measured by the DC method using a KEITHLEY 6517B Electrometer/High Resistance Meter (Keithley Instruments, LLC, Solon, OH, USA) and within the temperature range of 100-400 K. The thermoelectric power S(T), *i.e.* the Seebeck coefficient was measured within the temperature range of 100–400 K with the help of a Seebeck Effect Measurement System (MMR Technologies, Inc., San Jose, CA, USA).

Electrical conductivity measurements showed two areas: intrinsic in the temperature range of 350–400 K with strong thermal activation decreasing from E_{a1} ~1.5 eV for x = 0.0 to E_{a1} ~0.4 eV for x = 0.5 as well as extrinsic in the temperature range of 100–200 K, in which the weak thermal activation E_{a2} ~0.005 eV is observed (Table 1).

Table 1. Electrical parameters of $CuTa_{2-x}Sb_xO_6$ solid solution: a is the slope of the linear $S_{diff}(T)$ diffusion function of thermopower, E_F is the Fermi energy, T_F is the Fermi temperature (defined as E_F/k), k is the Boltzmann constant, E_{a1} and E_{a2} are the activation energies in the intrinsic and extrinsic regions, respectively.

x	a ($\mu V/K^2$)	E_F (eV)	T_F (K)	E_{a1} (eV)	E_{a2} (eV)
0	-0.374	0.196	2274	1.470	0.004
0.2	-0.439	0.167	1938	0.874	0.005
0.3	-0.466	0.157	1822	0.732	0.005
0.5	-0.481	0.152	1764	0.423	0.007

The temperature dependence of thermoelectric power, *S*(T), in conventional metals consists of two different parts, i.e. a diffusion component (S_{diff}), which according to the Mott formula [3] is proportional to temperature and a phonon drag component (S_{ph}), which is more complex. The experimental curve, *S*(T), can be easily fitted by the Matoba, Anzai and Fujimori semiempirical formula [4]:

$$S(T) = D \cdot T + E \cdot T^3 + \frac{F \cdot (\frac{T}{\theta_D})^3}{G + (\frac{T}{\theta_D})^4} + H \cdot T^{1/2},$$

where *D, E, F, G* and *H* are the curve-fitting parameters and θ_D is the Debye temperature. The diffusion contribution S_{diff} is a direct application of the Boltzmann transport equation [3], as follows: $S_{diff} = \frac{\pi^2 k^2}{e E_F} T = aT$, where *e* is the elementary charge, and *a* is an empirical slope.

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