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Temperature dependence of atoms mobility in Fe-Cr alloys studied by ^{57}Fe Mössbauer spectroscopy

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Motivation

Steel foil is an attractive candidate for use as a flexible substrate material for Cu(In$_x$Ga$_{1-x}$)Se$_2$ solar cells (CIGS). CIGS on stainless chromium steel foil with efficiency of 17.5% [1] belongs to the most efficient thin-film solar cells on flexible substrates. The main problem for steel foil substrates is diffusion of detrimental substrate elements, such as Fe or Cr, into the CIGS layer during the high temperatures processing, as they deteriorate CIGS cell efficiency [2, 3]. A great deal of understanding these diffusion processes can be achieved by studying simpler model systems such as Fe-Cr solid solutions. In this work we determine temperature dependence of atoms mobility in Fe$_{0.948}$Cr$_{0.052}$ alloy and estimate the temperature above which CIGS solar cells on stainless chromium steel foil cannot be processed and operate without loss of perfomance due to, mentioned above, diffusion of Fe and Cr atoms.

Experiment and results

The ^{57}Fe Mössbauer spectra were measured in transmission geometry by means of a constant-acceleration POLON spectrometer of standard design and using a 60 mCi ^{57}Co-in-Rh standard source with a full width at half maximum (FWHM) of 0.12 mm/s.

The measurements were performed for two kinds of Fe$_{0.948}$Cr$_{0.052}$ samples - thermal equilibrium ones being at several temperatures from 300K to 1100K as well as quenched ones. The latter samples were heated in argon atmosphere at different temperatures not exceeding 1050K, and then quenched into water being at about 295K in order to freeze the high temperature distribution of atoms. After the quenching process, each sample was chemically polished to remove possible surface contaminations. Some of the obtained spectra are presented in Figs. 1 and 2.

Each spectrum measured was fitted with a transmission integral for a sum of six different six-line patterns corresponding to unlike hyperfine fields B at ^{57}Fe nuclei generated by different numbers of Fe and Cr atoms located in the first two coordination shells of the probing nuclei. The fitting procedure was done under assumption that the influence of Cr atoms on B as well as the corresponding isomer shift IS of a subspectrum, is additive and independent of the atom positions in the given coordination shell of the nuclear probe although it can be different for atoms located in unlike shells.

As the main result of the analysis, effective thicknesses $T_A(n_1, n_2)$ of components for each spectrum were determined.

$$T_A(n_1, n_2) = \sigma_0 t_A N f c(n_1, n_2)$$

where σ_0 is the resonance cross section, t_A the thickness of the absorber, N the total number of resonant absorbing atoms ^{57}Fe per unit volume, $c(n_1, n_2)$ the fraction of absorbing atoms corresponding to the proper component and f the Lamb-Mössbauer factor. Assuming that the Lamb-Mössbauer factor is independent of the configuration of atoms in the surroundings of the ^{57}Fe nucleus, the effective thickness $T_A(n_1, n_2)$ is directly proportional to the relative fraction $c(n_1, n_2)$. Using the normalization condition
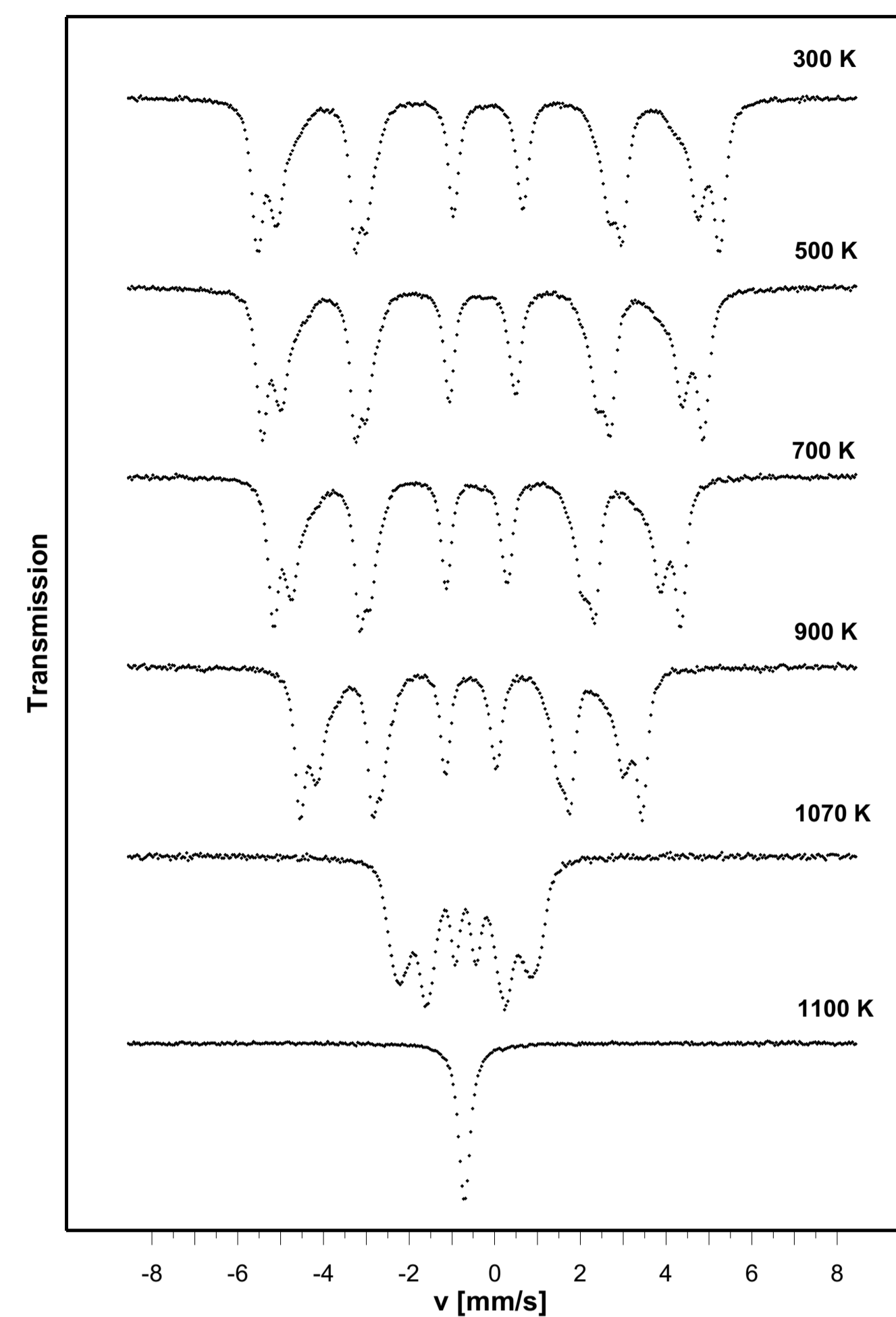
$$c(n_1, n_2) = \frac{T_A(n_1, n_2)}{\sum T_A(n_1, n_2)}$$

The computed $c(n_1, n_2)$ values were used to find parameters c_0, c_1 and c_2, being the total intensities of those components of a spectrum which are related to the existence of zero, one and two Cr atoms in the two first coordination shells of nuclear probes ^{57}Fe, respectively:
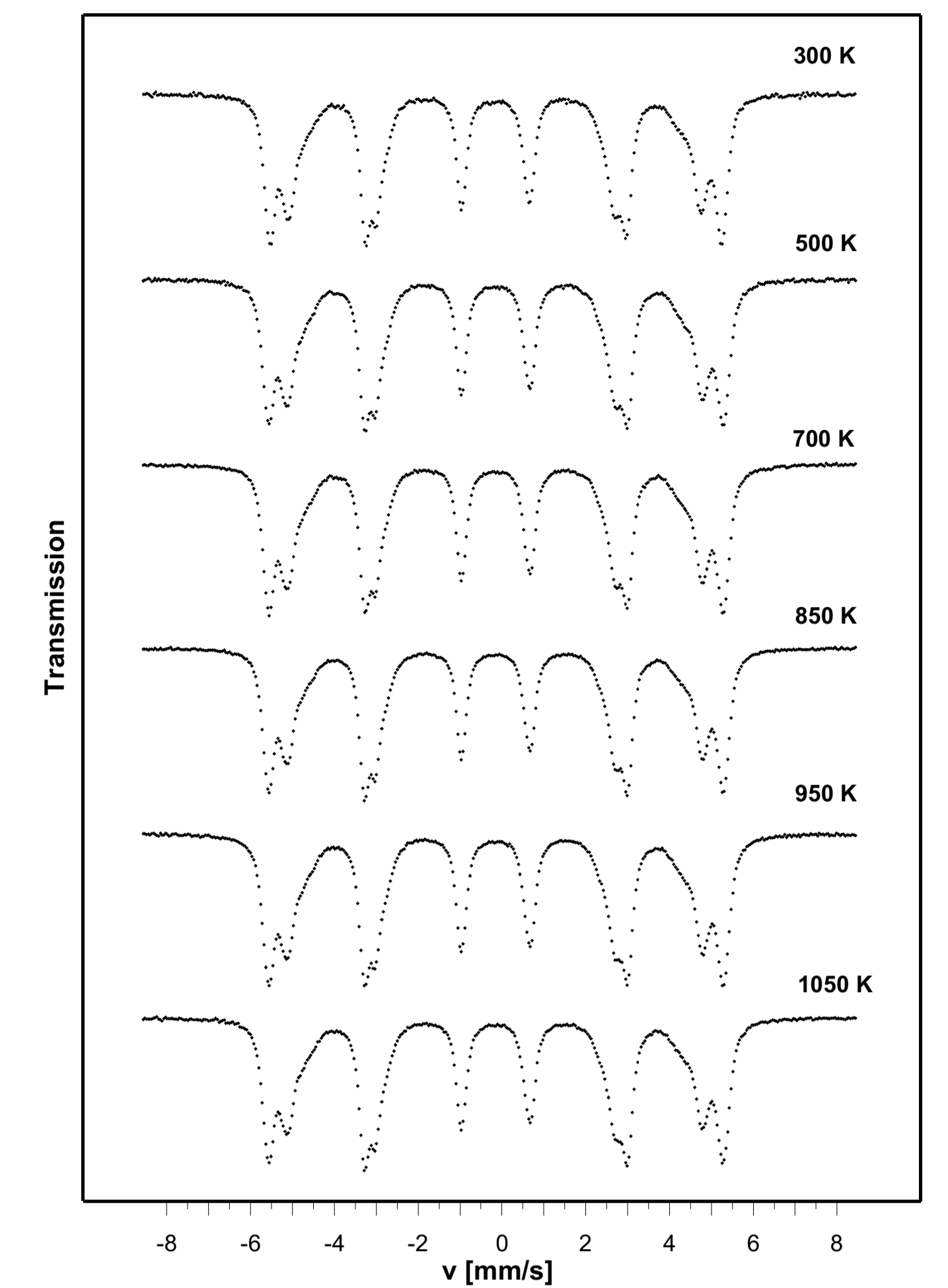$c_0 = c(0,0)$,
$c_1 = c(1,0) + c(0,1)$,
$c_2 = c(1,1) + c(2,0) + c(0,2)$.

Fig. 1 The ^{57}Fe Mössbauer spectra for the Fe$_{0.948}$Cr$_{0.052}$ alloy being at different temperatures.

Fig. 2 The room temperature ^{57}Fe Mössbauer spectra measured for samples of the Fe$_{0.948}$Cr$_{0.052}$ alloy quenched from different temperatures.

Fig. 3 The c_0, c_1 and c_2 parameters for the Fe$_{0.948}$Cr$_{0.052}$ alloy, being at different temperatures.

Fig. 4 The c_0, c_1 and c_2 parameters for the Fe$_{0.948}$Cr$_{0.052}$ alloys, quenched from different temperatures.

The measured spectra were analysed in terms of the c_0, c_1 and c_2 parameters, which characterize the atomic surroundings of the nuclear probes. The results are presented in Fig. 3 and Fig. 4. As one can see, the value of each parameter practically doesn't change with increasing temperature up to about 600-700 K which indicates a lack of atomic diffusion in the sample. On the other hand for higher temperatures there is a significant temperature dependence of the mentioned parameters which is an evidence that at these temperatures a diffusion of atoms in the specimen is possible. The temperature dependences of the c_0, c_1 and c_2 parameters were used for estimation of the "freezing" temperature T_d for the Fe$_{0.948}$Cr$_{0.052}$ alloy below which the diffusion of atoms in the material practically does not exist, assuming that each dependence $c_0(T)$, $c_1(T)$ and $c_2(T)$ can be approximated by two straight lines which cross each other when $T = T_d$. The equations of the lines were found by fitting them separately to the c_0, c_1 and c_2 values for temperatures T from two ranges 300 K - 700 K and above 700 K. The T_d determined this way amounts to 704(22) K for the thermal equilibrium sample and 659(108) K for quenched specimens.

Conclusions

From findings of the study it follows that the CIGS solar cells on stainless chromium steel foil should not be processed and operate at temperatures higher than about 650 K as it can lead to deterioration of the cell efficiency due to detrimental diffusion of substrate elements.
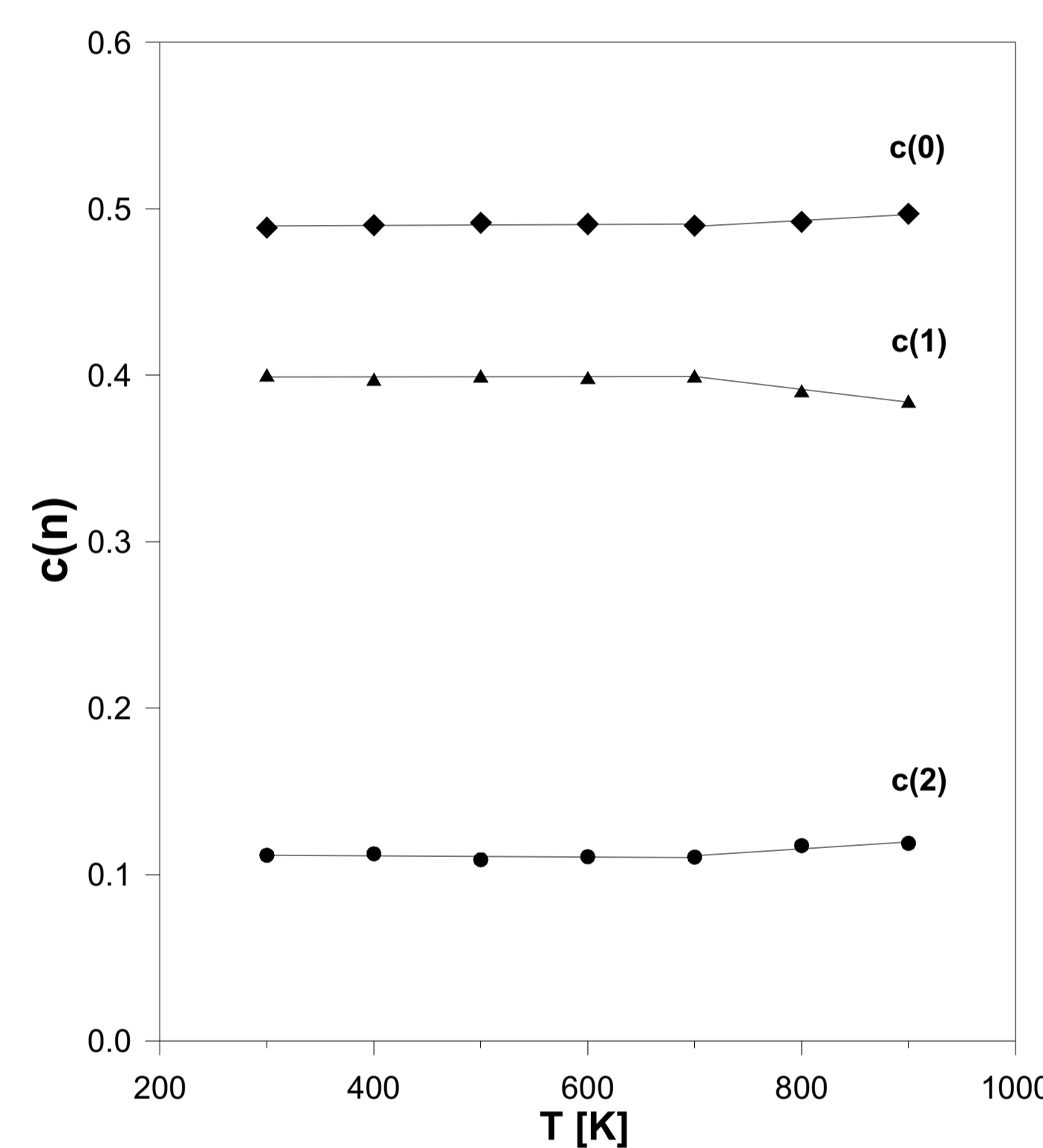
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[2] P. Jackson, P. Grabitz, A. Strohm, G. Bilger, H.W. Schock, in: Proceedings of the 19th European Photovoltaic Solar Energy Conference, Paris, France, 7 - 11 June 2004, p. 1936.
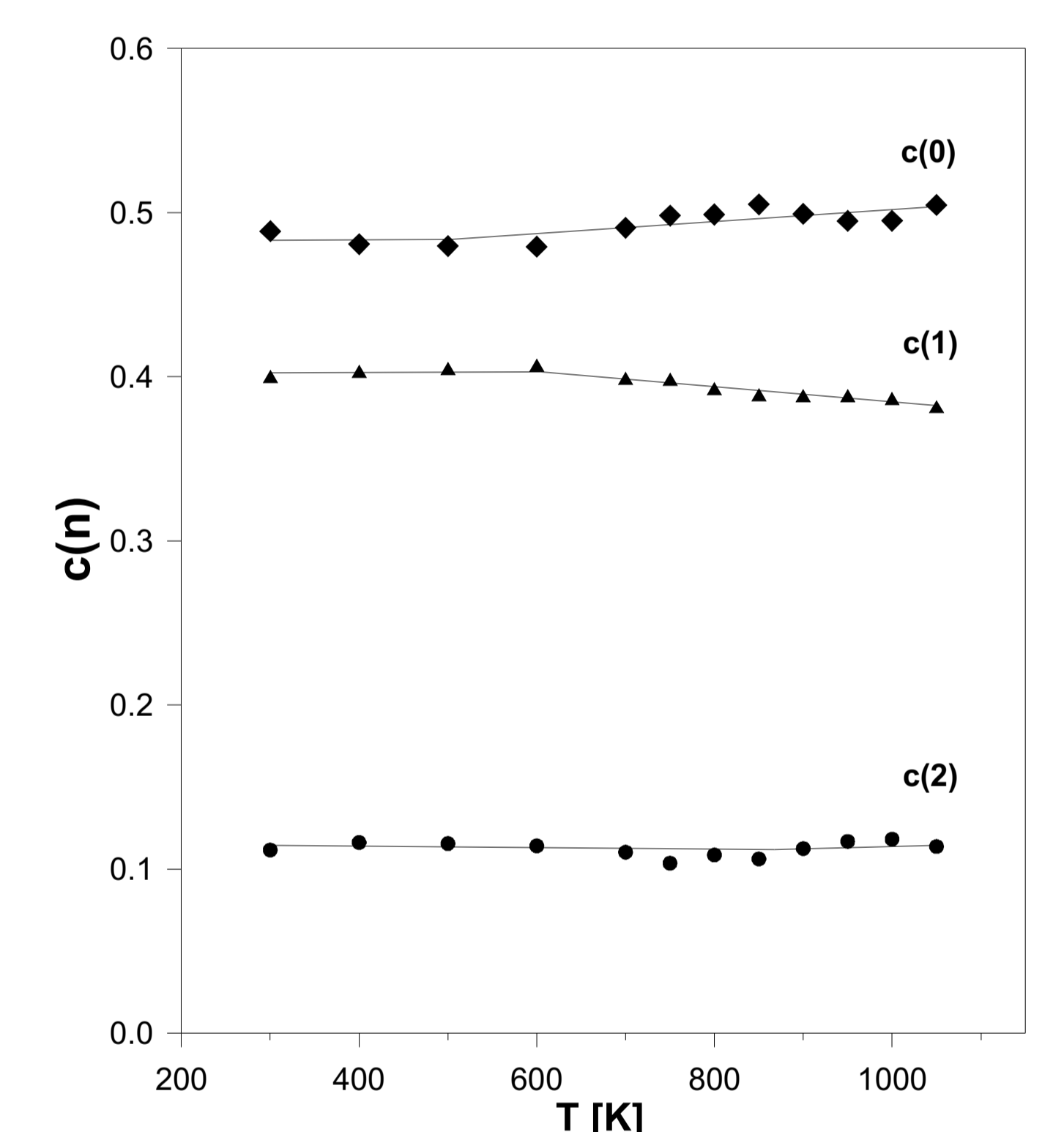[3] R. Wuerz, A. Eicke, M. Frankenfeld, F. Kessler, M. Powalla, P... Rogin, O. Yazdani-Assl, Thin Solid Films **517** (2009) 2415.