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# Modification of the reflectivity curve of GaTe in the Kramers-Kronig analysis

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According to the Kramers-Kronig (KK) analysis [1], the optical constants of GaTe have been determined from the normal-incidence reflectivity ($R$) data given in the range of 1.7–35 eV [2]. Unfortunately, the experimental $R$ curve required the modification in the range of 1.7–2.2 eV. The modification (Fig. 1) was necessary to obtain convergence in the cyclic algorithm and was attributed to the experimental error [2]. Recently, this attribution has been confirmed by the results obtained for the same $R$ data and for another algorithm of the KK analysis [3]. In that case a necessity of the $R$ curve modification was connected with the reasonable choice of the parameter value describing the high-energy $R$ extrapolation. However, no more detailed physical explanation of the neccessity of the $R$ curve modification has been found so far. The present work aims at reporting the study of this problem. In all the cases mentioned below, KK analysis was carried out in the way described in paper [3].

The experimental $R$ values of GaTe in the range of 20–35 eV are lower than $1\%$ [2]. These values of $R$ seem to be too low. If the experimental energy range is shortened up to 1.7–19 eV, the lowest $R$ values are avoided, and the KK analysis is performed for the $R$ given in this energy range. In this case no modification of $R$ curve is needed any more (Fig. 1). The low-energy $R$

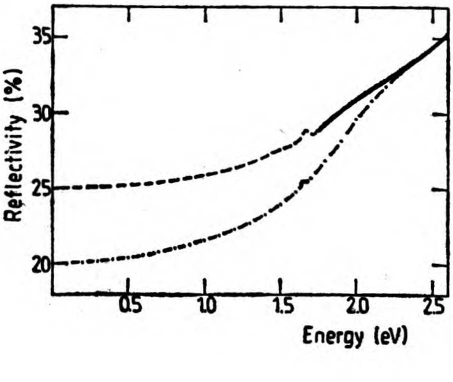


Fig. 1. Reflectivity curve of GaTe in the low-energy range with the extrapolation determined in the KK analysis: the experimental curve from the paper [2] – solid line, the extrapolation in the case of the KK analysis of the experimental data in the shortened energy range-dotted line, the extrapolation ncluding the modification of the experimental curve – dotted-dashed line

xtrapolation fulfills the continuity condition for $dR/dE$ at 1.7 eV, if the *average value* of reflectivity beyond the high-energy side of the measuring range is equal to $R_\infty = 0.007$. It is a reasonable value of $R_\infty$, because from the experiment it follows that the value of $R$ is equal to 0.02 at the last measuring energy point. It should be pointed out that when $R$ given in the range of 1.7–35 eV was analysed by means of the KK method, the value of $R_\infty$ was much greater than $R$(35 eV) and therefore the modification of $R$ curve mentioned above was required (for more details see [3]).

The fact that $R$ values are probably too low leads to the supposition that roughness of the sample surface can be considered as the cause of the necessity of the modification of $R$ curve. We assume that the measured values of $R$ are lower for a rough surface and we calculate the $R_0$ values for the ideally smooth sample in the range of 1.7–35 eV. The values of $R_0$ are obtained from the following formula [4]:

$$R/R_0 = \exp(-x^2)+[1-\exp(-x^2)][1-\exp(-B^2x^2/4)]$$

where $x = 4\pi SE/hc$, $B = \beta/m\sqrt{2}$, and $\beta$, $h$ and $c$ are a semivertex angle of the acceptance cone, Planck constant and velocity of light, respectively ($S$ and $m$ are the r.m.s. depth and r.m.s. slope of the roughness, respectively, $S$ and $1/m$ being equal to zero mean no roughness). We increase the values of these parameters untill no modification of $R_0$ curve in the range of 1.7–2.2 eV is required. The result of this procedure is not explicit, since roughness is described by two parameters. Therefore, first, we assume that $1/m$ is equal to zero, and next, that $1/m$ is relatively high ($m = 0.035$). Then the value of $S$ is determined. In the first case $S = 3.5$ nm is obtained, while in the other one $S = 12.5$nm. The reflectivity curves corrected for roughness and the measured one given for comparison are shown in Fig. 2. We would like to point out the fact

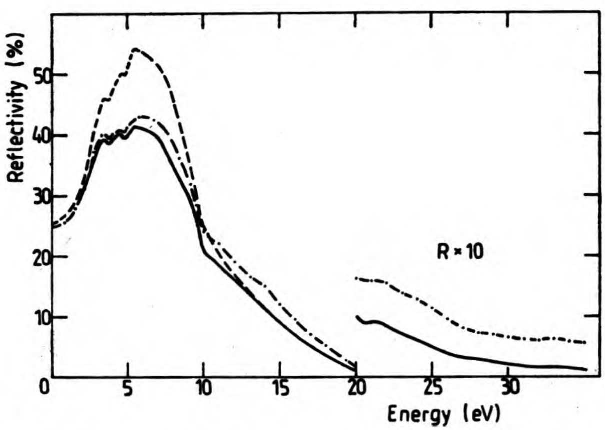


Fig. 2. Reflectivity curves of GaTe: the measured one from the paper [2] – solid line, and after correction for surface roughness – dashed line ($S = 12.5$ nm, $m = 0.035$) and dotted-dashed line ($S = 3.5$ nm, $1/m = 0$)

that the $S$ values obtained are in agreement with the experimental results of Czarnecka-Such and Kisiel [5]. Using Fringes of Equal Chromatic Order (FECO) method they determined $S = 11 \pm 2.5$ nm for the optical polished surface of Si. Such a surface was also investigated by Dash [6] who obtained the thickness of the strain layer of about 15 nm.

In summary, the KK analysis of the reflectivity data can produce unphysical results, such as necessity of the modification of the experimental $R$ curve considered in this paper and the dip in absorption coefficient curve [7]. If the determination of optical constants is carried out carefully, these features are connected with the experimental error only. Consequently, the efforts to avoid unphysical results provide information about the reasons of the experimental error. But then, more than one possibility can usually be found. In the case of GaTe we find that either the high-energy reflectivity is too low or the whole $R$ curve measured is distributed by roughness. The use of the formula cited provides estimation of parameters describing the roughness.

**References**

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