Some remarks on the paper “Optimization of S:Sn precursor molar concentration on the physical properties of spray deposited single phase Sn_2S_3 thin films”

by J. Srivind, V.S. Nagaretthinam, A.R. Balu [Mater. Sci.-Poland, 34 (2016), 393 – 398]

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The commented paper [1] presents the results of the structural, morphological, electrical and optical studies on thin film of orthorhombic Sn_2S_3 . Unfortunately, there are several mistakes or errors which should be revealed to avoid their use in the future papers by Authors and other people.

The main error is related to the way of the lattice parameters evaluation. Authors say that three independent lattice parameters of the orthorhombic unit cell, a , b and c , were calculated from only one diffraction peak, i.e. using one diffraction angle and one equation 1. It is not possible from the mathematical rules (one equation with three unknown values). Thus, the values of lattice parameters presented in Table 1 in the commented paper are totally wrong. One of the Authors (A.R.B.) explained this sensational procedure during personal contact. He used the “standard c/a ratio of orthorhombic crystal structure by approximation with the XRD data. From the estimated c and a values, b values are calculated.” The main problem is that such a standard c/a ratio does not exist for orthorhombic crystals. He wrongly supposed that c/a ratio known for some hexagonal crystals can be used

for orthorhombic species. Thus, the presented lattice parameters are wrong from the point of view of cited JCPDS Card, as well. The correct values are entirely different ($a = 8.87 \text{ \AA}$, $b = 3.75 \text{ \AA}$, $c = 14.02 \text{ \AA}$) comparing to those obtained in the commented paper: $15.5 \text{ \AA}$, $5.6 \text{ \AA}$ and $5.6 \text{ \AA}$, respectively (Table 1). This “deviation” from standard values was explained by the “approximation performed on the c/a ratio.”

One can find the interesting error in the formula for micro-strain evaluation, (3). It should be “ $\cot\Theta$ ” instead of “ $\cos\Theta$ ” ($\cot\Theta = \cos\Theta/\sin\Theta$). Unfortunately, this error is rather popular in other papers by the same authors’ team. This is a formula by Wilson for the broadening of diffraction profile due to microstrain existing within the sample. As a result, all data on the microstrain presented in Table 1 are wrong. If we use the correct function, $\cot\Theta$, the obtained values of microstrain are of about 3.5 times greater than those published in the commented paper.

It seems that the above errors have their source in the practice of citing only own previous papers instead of the original papers where some formula were used for the first time. Such self-citation leads to spreading of errors.

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There is a great discrepancy between the diffraction patterns shown by the Authors and SEM images from Fig. 2 in the commented paper. The X-ray diffraction suggests the single-crystalline character of the sample. However, the SEM images clearly indicate on the grains (flake- or needle-like) oriented in all directions without any specific preferred orientation suggested by the diffraction patterns. The only one explication is that the diffraction patterns were made on different samples than those studied by SEM.

In conclusion, the commented paper has many errors and presents wrong structural data.

Moreover, there are no evidences why the sample "0.02:0.02" can be treated as the thin film "with better physical properties." All presented data change gradually with the molar concentration. As a result this paper has a limited scientific value.

References

- [1] SRIVIND J., NAGARETHINAM V.S., BALU A.R., *Mater. Sci.-Poland*, 34 (2016), 393.

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