Formation of structural defects during Bi_2Te_3 epitaxy investigated by a Monte Carlo computational model

Celso I. Fornari[1]*, Gabriel Fornari[2], Paulo H. de O. Rappl[1], Eduardo Abramof[1] and Jerônimo dos S. Travelho[2]

National Institute for Space Research – INPE
[1] *Associate Laboratory of Sensors and Materials – LAS*
[2] *Associate Laboratory for Computing and Applied Mathematics – LAC*
*celso.fornari@inpe.br

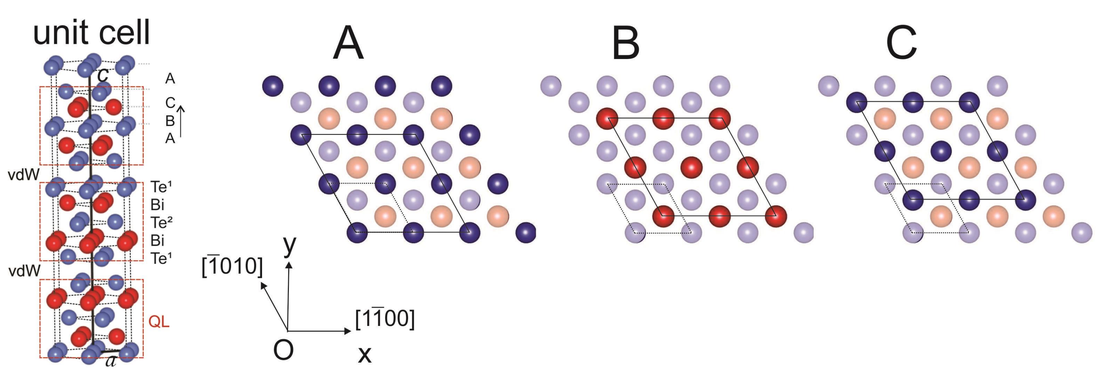
1. Introduction

Three-dimensional topological insulator materials have attracted great attention in scientific community in the past few years due to its extraordinary surface properties. However, the intrinsic presence of structural defects leads to bulk conduction, which overwhelms surface contribution from electrical measurements and results in an ordinary semiconductor material behavior. In this sense, several efforts have being employed to control the occurrence of these defects obtaining a truly bulk insulator behavior.

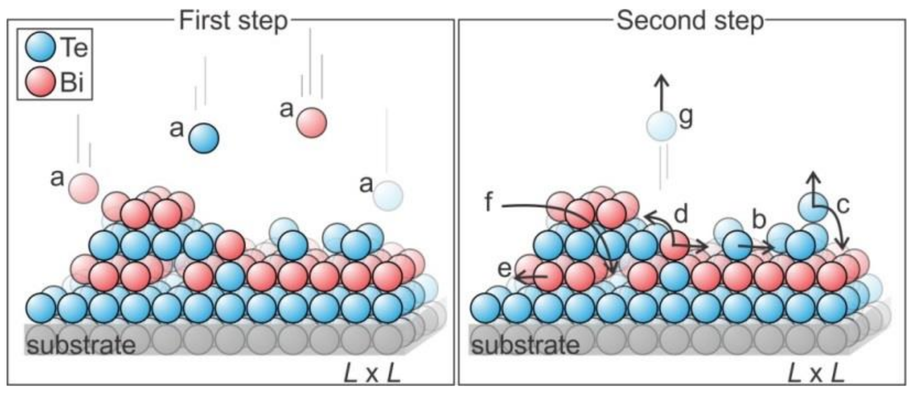
In this work a systematic investigation on the properties of the bismuth telluride epitaxial films is presented by using a Monte Carlo growth model. The model provides an atomistic understand on the growth dynamics and insights on the formation of structural defects.

2. Model

This model uses the nearest-neighbor and the lattice-gas approximations. A cubic lattice is used instead the hexagonal Bi_2Te_3 lattice, as previously adapted in other (111) and (001) Si computational models.



Each time round in the model is divided in two steps: the deposition of atoms and the surface analysis. In the first step, atoms are randomly deposited over the growing surface. In the second step, the probability of each event is computed.



The probabilities for diffusion (P_D) or desorption (P_E) are calculated based in an Arrhenius rate, defined as:

$$R_{D,E} = R_0 . \exp^{-\frac{E_{D,E}}{k_B T}}$$

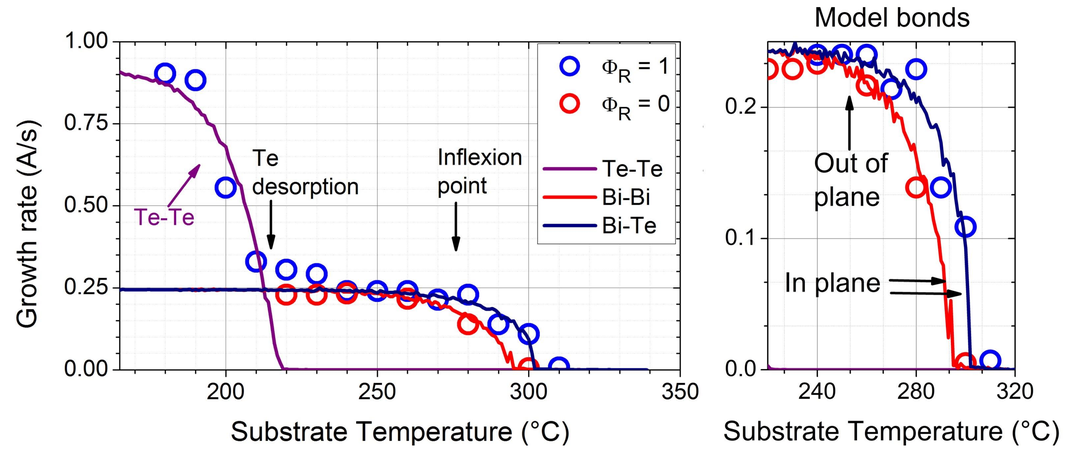
To accomplish the stochastic nature of the microscopic processes the 623 dimensionally equidistributed uniform pseudo-random generator Mersenne-Twister was used.

3. Results

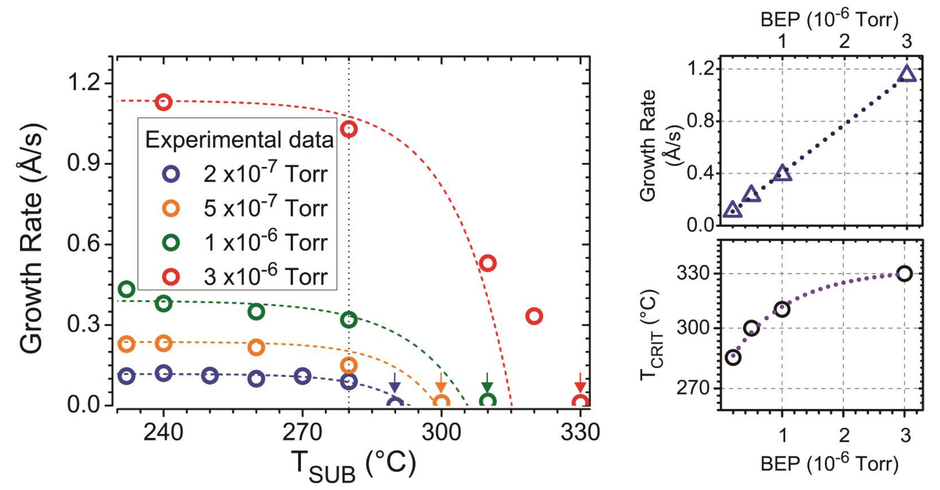
The energy barrier values for Bi and Te atoms in the model were fitted, using the lowest χ^2 values as parameter, to adjust the simulated growth rate curve to the experimental one.

For T_{SUB} up to 220°C all extra Te atoms sticks to the growing surface, as experimentally observed. Between 220 and 280°C a layer-by layer growth is achieved, with a film stoichiometry close to Bi_2Te_3. Above 280 °C the growth rate curves start to decrease, until certain critical temperature (T_{CRIT}) above which the films does not grow.

In the model, the out of plane energy determines the deflection point, i.e., the temperature in which the growth rate starts to decrease and the in plane energy determines the derivative of the decrement.

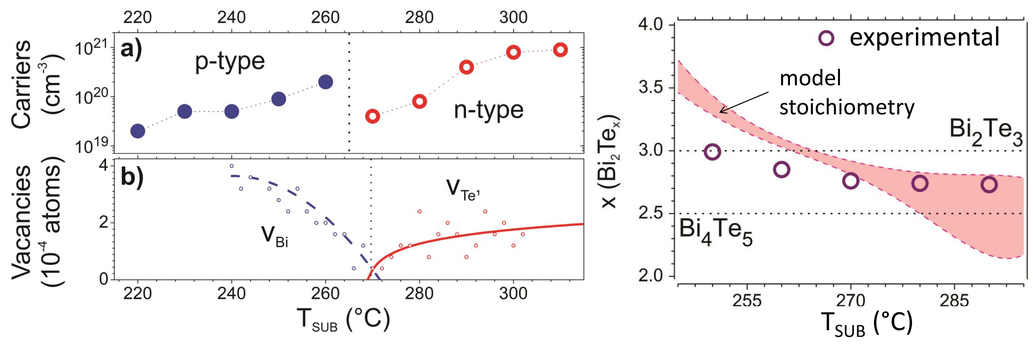


The BEP_{Bi2te3} is directly proportional to the deposition rate and T_{CRIT} depends exponentially on the BEP.



At low substrate temperatures the films present *p*-type carriers. By raising the substrate temperature up to 260 °C, the number of electrical carriers increases monotonically. For T_{SUB} = 270 °C, the films present suddenly *n*-type carriers, indicating a transition from holes to electrons as major carriers.

The computational model predicts the occurrence of bismuth vacancies in films grown at T_{SUB} lower than 270 °C. Close to 272 °C, the density of tellurium vacancies overwhelms the bismuth ones, increasing as T_{SUB} raises.



The Monte Carlo model predicts films with stoichiometry richer in Te than Bi_2Te_3 phase for T_{SUB} below 250 °C, while for films grown at higher T_{SUB} the model predicts Bi-richer phases than the experimentally observed.

4. Conclusion

A Monte Carlo epitaxial model was developed to study the growth of bismuth telluride compound. The results obtained here suggest that the model is in agreement to the experimental data, which indicates that the cubic lattice approximation can be used, as well as the the lattice-gas approximation.

The *p* to *n* transition is qualitatively explained by the computational model. However the computational model predicts Bi-richer phases than experimentally observed, which can be an indicative of incorrect barrier energy values for lateral bonds.

Acknowledgments

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