Advances in Modeling of the Bulk Crystal Growth & Epitaxial Thin Films

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In response to the technology developments and customers' demands to reduce manufacturing time for a faster market entry, alternative solutions are provided by using mathematical skills and computational techniques, e.g., automated software to assist and optimize product requirements, virtual prototyping, etc. In addition, advanced energy technologies catalyze transition to a new era of "inverse design" where the desired properties of materials drive the rapid exploration within advanced computing at the atomic scale and new algorithms to accelerate materials discovery.

This talk refers to both approaches: (i) the advances in modeling of bulk materials grown from the melt without contact with the crucible walls – research performed in collaboration with international experts from Europe; and (ii) first-principles theoretical investigations on some new perovskites synthesized epitaxially at the Ferroic Lab from INRS-EMT, Canada.

First, qualitative and numerical studies are presented for Young-Laplace equation of the liquid meniscus surface in the case of Czochralski (CZ), edge-defined film-fed growth (EFG), Dewetted Bridgman. Then, nonlinear dynamical systems describing the crystal size and meniscus height are discussed, together with optimization of crystal growth process parameters and control of the crystal shape. Further, compositional uniformity is predicted for EFG cylindrical bars using the system of partial differential equations that describes heat, momentum and mass transfer, as well as effect of the Marangoni forces.

Regarding epitaxial thin films, their properties are strongly related to the material crystal structure, and hence it is sometimes difficult to discriminate between the various phenomena observed on the sole basis of experimental data. To provide extensive insight into electronic properties, magnetic orderings, distortions and ferroelectric properties of the double perovskites $A_2MM'O_6$ (M has partially filled e_g-orbitals, and M' has empty e_g-orbitals), DFT simulations are performed using the projector-augmented wave (PAW) formalism within *Vienna ab initio Simulation Package* (VASP). Exchange and correlation effects are treated using the local density approximation plus Hubbard potential total-energy functional approximations (e.g., LSDA+U, GGA+U), for different possible high spin (HS) and low spin (LS) configurations using both collinear and non-collinear spin polarized calculations. Effect of spin-orbit coupling (SOC) is investigated, magnetocrystalline anisotropy energy is computed, and the easy axis corresponding to the saturated magnetic moment is determined.