

Modeling and numerical simulations of microwave-induced ionic transport

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(Received 24 September 1997; accepted for publication 24 February 1998)

A numerical model was developed to simulate and study microwave-induced transport in ionic solids. The model is based on continuum equations, is very general, and could be applied to many materials. The assumptions, boundary conditions, initial conditions, and numerical techniques used in the model are described. Results are presented from a study of microwave driven defect transport in sodium chloride. Static, high-frequency, and quasistatic results show that ponderomotive rectification of vacancy fluxes will act to deplete the vacancies in a near-surface region and will continue to pull vacancies to the surface through diffusion kinetics. The ponderomotive driving force for this transport is characterized over a wide range of variable space. The magnitude of the driving force falls right in the range such that it can explain why microwave-enhanced mass transport is observed in some experimental cases but not in others. © 1998 American Institute of Physics. [S0021-8979(98)02311-1]

I. INTRODUCTION

The heating of a material depends on two physical processes. First, energy must be absorbed and converted to heat through high-energy gas particles colliding with the surface of the material (convection heating) or via an interaction between the material and electromagnetic fields (radiation heating). Second, the absorbed heat will transfer within the material via electron or phonon energy transfer (thermal conduction). High-temperature heating of ceramic materials usually involves heating the surface of the sample with infrared radiation, but heating rates are limited by the slow rate of inward heat conduction due to the typically low thermal conductivities of ceramics. Microwave radiation, on the other hand, penetrates deeper, allowing for more volumetric heating and relying less on thermal conduction.

Microwave heating has niche applications for materials with certain absorption and thermal conduction properties, and many ceramic materials fall into this category. In recent years, many researchers have studied high-temperature microwave processing of ceramics such as firing, sintering, joining, and melting.¹ The initial stimuli for their efforts were the unique benefits that microwave heating might provide that conventional heating could not. These anticipated benefits included more precise and controlled volumetric heating, faster ramp-up to temperature, lower energy consumption, and improved quality and properties of the processed material.

Besides the anticipated benefits, many experimenters have also observed an apparent “nonthermal” effect in the

form of enhanced kinetics. Specific observations in ceramic materials include enhanced rates of sintering,^{2,3} grain growth,⁴ surface-penetration diffusion,^{5,6} joining,^{7,8} and nucleation.⁹ There is also much anecdotal evidence for microwave enhancements of polymer processing, epoxy curing, catalysis, and reactions in organic materials.

An important recent breakthrough in the understanding of these empirical observations has been the identification of a fundamental mechanism which nonthermally enhances solid state ionic mass transport. This previously unrecognized phenomenon^{10,11}—articulated as a “ponderomotive force” (*pmf*)—is now understood to be a fundamental property of microwave-irradiated interfaces that represent abrupt discontinuities in ionic mobility. Microwave-excited ionic currents become locally rectified (near the interface), giving rise to an additional driving force for mass transport. Preliminary experimental evidence for the action of the microwave ponderomotive force was first reported,¹² and subsequent confirmation was realized by experimental observation of very specific, theoretically predicted transient decay dynamics of *pmf*-induced ionic currents in halide salt crystals.¹¹ From a mathematical standpoint, microwave ponderomotive forces at material interfaces are explicitly revealed upon nonlinear perturbation analysis of three fundamental equations applied to a material interface or surface: the continuity equation, Gauss’s Law, and the mass transport equation for mobile ionic species. This is discussed in greater detail in the body of this paper. A critical point to emphasize, however, is that no additional model-specific assumptions are needed to derive the existence of the microwave *pmf* from the three quoted equations from which it is derived; it can be active for crystalline (Schottky or Frenkel disorder) or amorphous microstructures.

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