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A detailed study on melting dynamics influenced by the pulse laser-induced transient heating

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ABSTRACT

This paper presents a detailed study on the melting dynamics induced by the pulse laser heat transfer process. A numerical model has been developed in an open-source based computational fluid dynamics (CFD) platform, known as OpenFOAM. Upon development, its predictions have been compared with the experimental results of nanosecond pulse laser annealing of silicon with a pulse duration of 30 ns and wavelength (λ) of 308 nm, in which an excellent agreement with the experimental results for both of the melt depth and the melting duration has been observed. In the second part of this study, the numerical model has been implemented to explain the pulse laser-induced melting dynamics of silicon wafers irradiated with KrF excimer laser, which is similar to the cases used for processing of industry compatible photovoltaic solar cells. Since the results explain how thermal process, induced by the transient energy, controls the propagation of melting dynamics, this contribution can be used as a guide for designing new laser systems as well as optimisation of a chosen application.

1. Introduction

Material modifications by means of pulse lasers are the most interesting methods used in the processing of various photovoltaic as well as electronic devices. They offer the ability to provide spatially precise and localised heating on potentially short timescales and offer continuous, high throughput, in-line processing. Under suitable conditions, the heat treatment associated with the pulse laser processing results in a phase-change process in the near surface region of the irradiated material. The basic sequence that occurs is always the same: melting of the near surface region and redistribution of atoms in the melt, followed by rapid solidification. This enables a number of applications to be performed such as dopant diffusion [1–8], junction formation [5,7,9–11], and damage removal from the ion-implanted layer [1,5]; which are considered as the key applications in processing of high efficiency devices, notably in the cases of photovoltaic solar cells processing.

For such applications, it is important to achieve well control on the melting process. The melting process is typically characterised by the melting parameters such as melting duration, melt depth, and re-solidification velocity. Inappropriate settings of these parameters can result in non-optimal process outcomes [4,7,12–19]. It has been reported that a number of defects can be generated during the laser processing if the melting parameters are not well controlled [4,2]. The reported defects are mostly generated from the quenching process due to the fast cooling and re-solidification of the irradiated layer and are concentrated in the vicinity of the surface layer [4,2]. Additionally, the fast heating process combined with the limited thermal conductivity of liquid phase creates a spatial temperature gradient not only at the surface but also in the deeper region of the material. This temperature gradient eventually enhances the formation mechanical stress in the material [20]. Moreover, in many cases, the melting process requires prolonged melt duration without vaporisation of the materials [21]. Although final result of the melting process can be controlled by a number of laser irradiation parameters, the transient heating induced by the temporal distribution of pulse intensity, has the most substantial effects on the melting dynamics. This is because changing the heat distribution within a single pulse can completely change the melting behavior. Hence, a clear understanding of how the melting dynamics are controlled by the pulse laser-induced heat transfer process is absolutely necessary. Understanding of the heat transfer process has another importance as it can result in brittleness, hardness and crack damage of the surface, and thermally induced mechanical stress within the wafer if the temperature is not well controlled. In addition, to optimise a chosen application and/or new laser developments, it is also necessary to analyse and

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characterise the thermal effects associated with the laser pulse.

To obtain the understanding of the induced heat transfer and phase change required for the controlled melting process as well as designing and optimisation of pulse shapes, experimental or numerical methods could be employed. Experimentally, there are several studies on pulse laser-induced melting which report the final outcomes in terms of the resulting material properties after the laser processing [22], however, without fully understanding the reasons behind those outcomes, optimal outcomes are not guaranteed. There have been a few attempts to experimentally measure important parameters during the process of pulse laser-material interaction, such as surface temperatures [23,24], surface phases [22], melting depth and duration [25] etc. While valuable, these measurements are quite difficult and typically only measure quantities at the surface; therefore they are unable to explain quantities of interest such as re-solidification velocities, internal cooling rates, etc.

Numerical approaches offer a valuable alternative. Several relevant numerical studies of melting and solidification during pulsed laser material interactions have been reported. Most relevant to the present contribution can be stated as Matsuno investigated the effect of pulse duration [9] on the melting depth, Gonda et al. [26] and Hackenberg et al. [27] investigated the effect of pulse repetition on the melting depth and duration, the effect of substrate heating on the re-solidification velocity was examined by Young et al. [7], Aziz et al. [28] investigated the effect of wavelength on the melting depth and duration, Cole et al. [29] examined effect of laser power on the melting depth, and the melting of films, as well as substrates, were examined by Font et al. [30] and Trice et al. [31].

However, none of these studies conducted a detailed study on understating the melting dynamics induced by the thermal process of pulse laser annealing. As already noted, a complete understanding of the thermal process potentially offers control on the melting parameters as well as designing and optimisation of the pulse shapes. This, therefore, motivates the present numerical study on explaining the melting dynamics induced by the thermal process.

2. Objectives and problem descriptions

In view of the above background, the objectives of this contribution are to investigate how the melting dynamics are influenced by the transient thermal process. To do so, a practical manufacturing case of processing silicon wafers for photovoltaic solar cells is chosen. In this case, the pulse laser in the nanosecond regime is used to heat and hence conduct melting and solidification of silicon wafers, which eventually enables laser doping of the wafers.

In setting up the problem, it is considered that the silicon wafer is heated by a nanosecond KrF excimer laser, which is often used for processing of silicon wafer-based solar cells [32–35], having a wavelength of (λ) of 248 nm. The laser power density is constant over the considered surface; which in turn reduces the problem to be solved in one-dimension. On the contrary, the temporal shape of the laser pulse is taken as Gaussian with a full width at half maximum (FWHM) of 32 ns. The laser fluences are chosen low enough so that the vaporisation temperature of silicon would not be reached, which is one of the major criteria in the laser doping process.

A schematic of the problem modelled in the simulation is presented in Fig. 1(b). The laser is assumed to be normally incident on the surface. The melt front is directed inwards of the wafer and considered as positive, whereas the solidification velocity is considered as negative in the chosen coordinates.

3. Numerical procedures

3.1. Governing equations

To obtain the temperature field and capture the propagation of melting front due to laser irradiation, an energy-based formulation of the heat conduction equation, taking into account the enthalpy of melting and solidification, was used. The energy-based formulation of the heat conduction equation may be written as [36],

$$\frac{\partial H}{\partial t} = \nabla.\,(K\nabla T) + Q_{laser}, \tag{1}$$

here, H is the total enthalpy, K is the thermal conductivity, and Q_{laser} is the heat source due to the absorbed laser power which can be expressed as,

$$Q_{laser} = (1-R)\alpha I. \tag{2}$$

Here, R is the reflection coefficient, α is the absorption coefficient, and I is the laser beam intensity. The laser beam intensity I can be calculated resolving the absorption equation, which can be expressed as,

$$\frac{\partial I}{\partial y} = -\alpha I. \tag{3}$$

The total enthalpy in the energy equation, Eq. (1), consists of the sensible enthalpy and the latent heat of fusion when melting and solidification is considered. Therefore, H may be expressed as [36],

$$H = h + \gamma\rho L_f = \int_{Tref}^{T} \rho C_p \partial T + \gamma\rho L_f. \tag{4}$$

Here, h is the sensible enthalpy, L_f is the latent heat of fusion, T_{ref} is the reference temperature, C_p is the specific heat, ρ is the density, and γ is the phase fraction. Substituting Eq. (4) into Eq. (1) leads to the following form of the energy equation,

$$\frac{\partial(\rho C_p T)}{\partial t} = \nabla.\,(K\nabla T) + Q_{laser} - \rho L_f \frac{\partial \gamma}{\partial t}. \tag{5}$$

The liquid fraction in the energy equation, Eq. (5), is a Heaviside step function which may be written as,

$$\gamma = 1,\ \text{when } T > T_M,\ \text{and} \qquad \gamma = 0,\ \text{when } T < T_M, \tag{6}$$

where, T_M is the melting temperature. To complete the mathematical description of the problem, the boundary and initial conditions are specified. Since the effect of both convective and radiative heat transfer from the front surface, y = 0, is negligible [18], the Neumann boundary condition may be used. At the bottom of the wafer, y = d, the Dirichlet boundary condition may be employed, as the wafer is thick enough to act as a good heat sink and temperature at the bottom of the surface remains unchanged. Here, d is the depth of the wafer. Note that, since the wafer is working as a heat sink, the heat losses will be driven by the conduction losses within the wafer and hence the losses due to convection and radiation will be negligible at the front surface, i.e. y = 0, in both of the solid and liquid phases. Therefore, the initial and boundary conditions for the problem may be summarised in the following,

$$T(y,0) = T_0, \tag{7}$$

$$-K\frac{\partial T}{\partial y}|_{y=0} = 0,\ \text{and}\ T(d,t) = T_0, \tag{8}$$

here, T_0 is the initial temperature.

3.2. Solver development in OpenFOAM

The mathematical models described in Section 3.1 are solved by developing a numerical model in OpenFOAM, which uses the finite volume method (FVM) in discretisation of the governing equations. Like other FVM suites, in OpenFOAM, the problem domain is decomposed into control volumes, and then the integral balance equations are formulated for each of the control volumes. The approximation of integrals by numerical integration, and function values and derivatives by interpolation with the nodal values lead to a system of algebraic equations, which are solved to get the final results. The details of the