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Molecular Dynamics Simulation of surface vaporization in beryllium Plasma Facing Components

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Abstract

An important feature of beryllium is its high vapor pressure. Small fluctuations in beryllium vapor pressure produce non-negligible differences in thermal behavior of Plasma Facing Components under high heat flux exposure, during off-normal events and Edge Localized Modes.

On the basis of an available pair potential, classical Molecular Dynamics (MD) Simulations have been carried out in order to evaluate beryllium vapor pressure and latent heat of vaporization under tokamak conditions.

Results from Molecular Dynamics Simulations show a good agreement with the experimental value for the latent heat of vaporization. Vapor pressure, evaluated through Clapeyron's equation on the basis of simulations results, is affected by more uncertainties and shows a poor agreement with the available experimental data.

Keywords: Plasma Facing Materials; Thermal erosion; Molecular Dynamics

1. Introduction

The erosion of the First Wall is a critical issue that could affect the performance and the operating schedule of the nuclear fusion reactor ITER. Primary effects ensuing from erosion/redeposition include plasma contamination, reduction of components lifetime, dust, and formation of mixed-materials, whose behavior is still uncertain [1]. Plasma Facing Component (PFCs) damage, due to high temperature excursions during off-normal events and Edge Localized Modes (ELMs), remains a critical issue. The strong overheating, in fact, produces material ablation through vaporization, melting and possible loss of molten material.

The aims of this work are the evaluation of the evaporative flux and the determination of beryllium latent heat of vaporization, in order to better predict the thermal behavior and the erosion of beryllium tiled PFCs in fusion devices.

Beryllium is the candidate material for the First Wall in ITER, whereas tungsten is the preferred material

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for the divertor. Carbon fiber composite could be used for the area of the divertor near the strike points. The choice of different materials depends on the specific operational requirements [2].An important feature of beryllium is its high vapor pressure. During thermal transients the strong vaporization keeps surface temperature relatively low but eroded thickness results high as well. Small changes in beryllium vapor pressure produce non-negligible differences in thermal analysis results.

The availability of increasing computational resource and accurate potential laws for different materials makes Molecular Dynamics (MD) Simulations a powerful tool for evaluating material physical properties. On the basis of an available interatomic potential [3], classical Molecular Dynamics Simulations have been carried out in order to evaluate beryllium vapor pressure and latent heat of vaporization under tokamak conditions.

2. Model for surface evaporation

The model used to evaluate surface evaporation in PFMs refers to existing models developed to describe laser ablation in metals [4,5]. When the evaporative flux is not too high, atoms leaving the heated surface do not collide and their velocity distribution is well described by a half-Maxwellian [5]. The flux Φ_s of evaporating atoms is thus given by the following expression:

$$\Phi_s = n_s \sqrt{\frac{k_B T_s}{2\pi m}} \tag{1}$$

where n_s is the atom density of vapor, T_s is the surface temperature, k_B is the Boltzmann constant, and m is the atom's mass.

The atom density n_s is related to the surface temperature and the vapor pressure p_s through the perfect gas law [4]. Vapor pressure can be evaluated, in turn, by means of the Clapeyron's relation, as an exponential function of the heated surface temperature T_s:

$$\frac{dp_s}{dT_s} = \frac{H_{vap} m}{T_s(v_g - v_f)} \tag{2}$$

where v_g and v_f are, respectively, the specific volume of vapor and liquid. Neglecting the liquid volume with respect to vapor volume and assuming vapor phase to be adequately described by perfect gas law, Eq. (2) can be easily integrated, yielding vapor pressure as a function of temperature.

The resulting evaporative flux $q''_s(T_s)$ is:

$$q''_s(T_s) = \sqrt{\frac{1}{2\pi m k_B T_s}}\, p_0\, e^{-(H_{vap})/(k_B T_s)} H_{vap} \tag{3}$$

where p_0 is a reference pressure and H_{vap} is the latent heat of vaporization per atom.

Increasing the evaporation flux results in a non-negligible collision rate among the evaporating atoms. The velocity distribution changes moving away from the surface, leaning toward an equilibrium condition. The distribution at equilibrium is still a Maxwellian with a non-zero mean velocity [5]. The region between the heated surface and the equilibrium point is called Knudsen layer and has a thickness of the order of the atoms mean free path [5]. Due to collisions, the evaporating atoms are partially back-scattered and a fraction of the emitted vapor condenses. The fraction of the emitted evaporative flux which back-condenses is ~20% and can be evaluated imposing mass, momentum and energy balances.

The vapor cloud expands across magnetic field lines and is heated and ionized by the incoming plasma. The interaction between plasma and vapor cloud could strongly reduce the heat flux which reaches the component surface and the overall erosion may strongly decrease [6]. The effect of vapor shielding is still uncertain, however, because of the potential instability and dispersion of vapor cloud [1,6]. The grazing angles between magnetic field and Be tiles in First Wall may promote vapor cloud instability.

Rather different correlations are available in literature for computing beryllium vapor pressure as a function of the surface temperature [7,8]. Fig. 1 shows that the evaporative flux is much sensitive to uncertainties in beryllium vapor pressure and that the effect of back-condensation is comparatively smaller.

Molecular Dynamics Simulations have been employed in order to evaluate the latent heat of vaporization in beryllium and to understand which parameters mainly affect vapor pressure fluctuations.