

## First-principles study on surface atom evaporation under electron field emission

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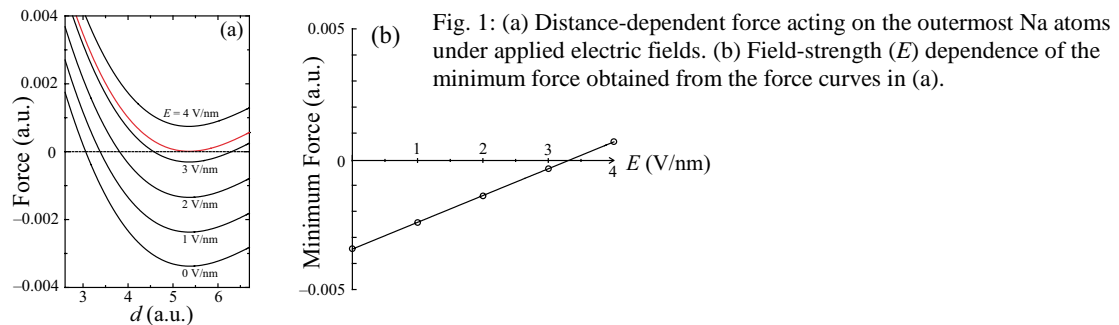
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Field emission (FE) is a quantum-mechanical electron-tunneling phenomenon from a tip surface with a high curvature to vacuum that accompanies high electric field and electric-current density. Such high fields and current densities tend to reconstruct the atomic geometry at the tip or even destroy the tip surface.<sup>1,2</sup> The stability of the tip surface is of critical importance for applications since it determines the lifetime of the field emitters.<sup>3</sup> However, the mechanisms of these surface structural changes during FE have not yet been understood, because there have been few studies thus far on the microscopic analysis of forces acting on surface atoms in the presence of electron emission.<sup>4</sup> Our objective in this study<sup>5</sup> is to explore FE-assisted surface evaporation.

We investigate Na (001) surfaces on the semi-infinite jellium electrode using the recursion-transfer-matrix (RTM) method<sup>6,7</sup> based on the density-functional theory. The whole system in the RTM method is divided into three regions; electrode, surface and vacuum regions. In solving Kohn-Sham equations in the surface region with some atomic structures, scattering waves are obtained by connecting to plane waves at the surface-electrode boundary and to Airy functions at the surface-vacuum boundary. The Airy functions are the solutions of Schrödinger equations under an electric field in one dimension.

Figure 1 shows the force curves under applied fields in the model with triple Na layers. A positive value of the force denotes the force direction away from the surface.  $d$  represents the distance between an outermost Na layer and the neighboring one. We observe two features in Fig.1(a). The first is that a threshold electric field  $E_{th}$ , beyond which the Na atoms can evaporate without an energy barrier, exists between 3 and 4 V/nm.  $E_{th}$  is determined with good accuracy by interpolating the values of the minimum force as a function of the electric-field strength  $E$ , as shown in Fig.1(b). The value of  $E_{th}$  obtained is 3.3 V/nm. The force curve for the  $E_{th}$  value is indicated by the red curve in Fig.1(a). The corresponding FE-current density is 0.018 nA/nm<sup>2</sup>. The second observation relates to the electric-field dependent equilibrium position  $d_{eq}$ . The  $d_{eq}$  value, at which the force is zero, is found to increase (i.e., the stable position of Na atoms moves towards the vacuum) with increasing  $E$  from Fig.1(a).

In the presentation, we interpret these properties from the potential energy. We also discuss common features between the Na-atom evaporation obtained here and usual field evaporation.



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