Probing Surface Structure through CO Diffusion on Cu(410)

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We discuss the possibility of using adsorbed CO for adsorbate mediated surface analysis. CO is known to exhibit properties that depend strongly on the local environment, e.g., coordination on surface sites, which manifest through its vibrational frequency. This, in turn, suggests the possibility of probing the surface structure through the changes in C−O stretching frequency during surface diffusion. Using density functional theory calculation, we demonstrate that the vibrational frequency shifts of CO manifests the corrugation of the surface, hence, its structure (cf., Fig.1). To show this, we used Cu(410), a wide stepped surface, as our sample.

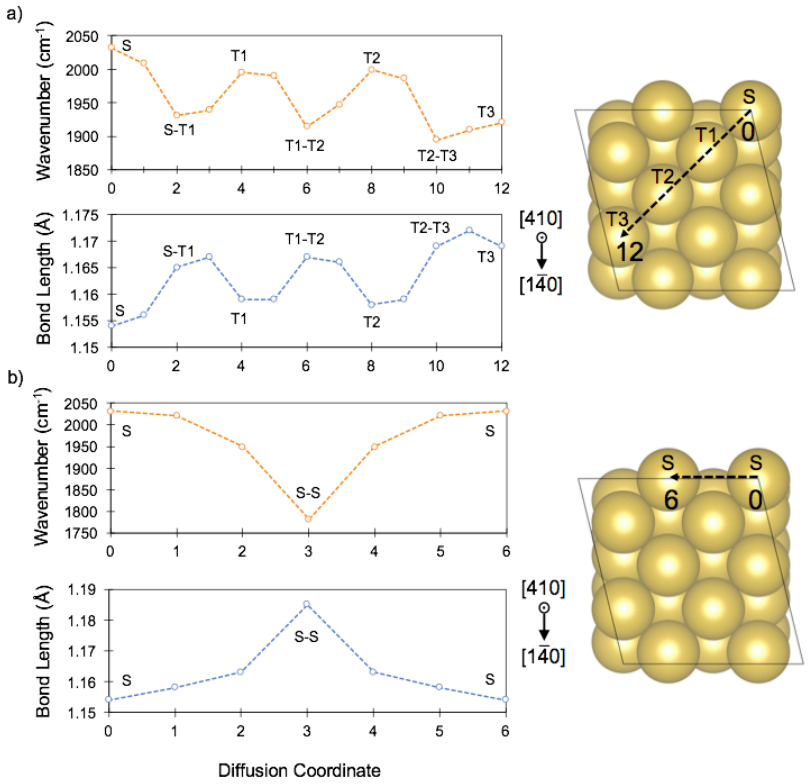

Fig. 1. Wavenumber (orange) of C-O stretching and its corresponding bond length (blue) for diffusion along a) the (100) terrace and b) step edge.[1)]

Reference:

1. J.S. Gueriba, N.B. Arboleda Jr., W.A. Diño, CO Diffusion and Bond Weakening on Cu(410) –Probing Surface Structure–, e-J. Surf. Sci. Nanotechnol. 18 (2020) 307-311.