Theory of Auger decay for fine surface structure features. GIAN PAOLO BRIVIO, Universita’ di Milano-Bicocca, MARIO ITALO TRIONI, INFM, SEBASTIANO CARAVATI, Universita’ di Milano-Bicocca — We calculate the core-core-valence (CCV) Auger profiles of an adatom on a periodic surface within the DFT framework by using a method based on the local density of states (LDOS), with a core hole on the atom, in the neighbourhood of the impurity. We investigate the CCV lineshapes of Na on Al(111) for the two ordered phases observed at room temperature. From a detailed comparison of the calculated spectra with specific recent experiments for the KL$_{23}$ lineshape of Na, we prove that a theoretical effort (based on DFT) can allow for determining the fine details of the two surface geometries of the adsorbate system, and also for unravelling components from inequivalent adatoms coexisting in the signal.