Electronic Supplementary Material (ESI) for RSC Advances.

Electronic Supplementary Information of "Molecular dynamics simulations of the initial oxidation process on ferritic Fe-Cr alloy surface"

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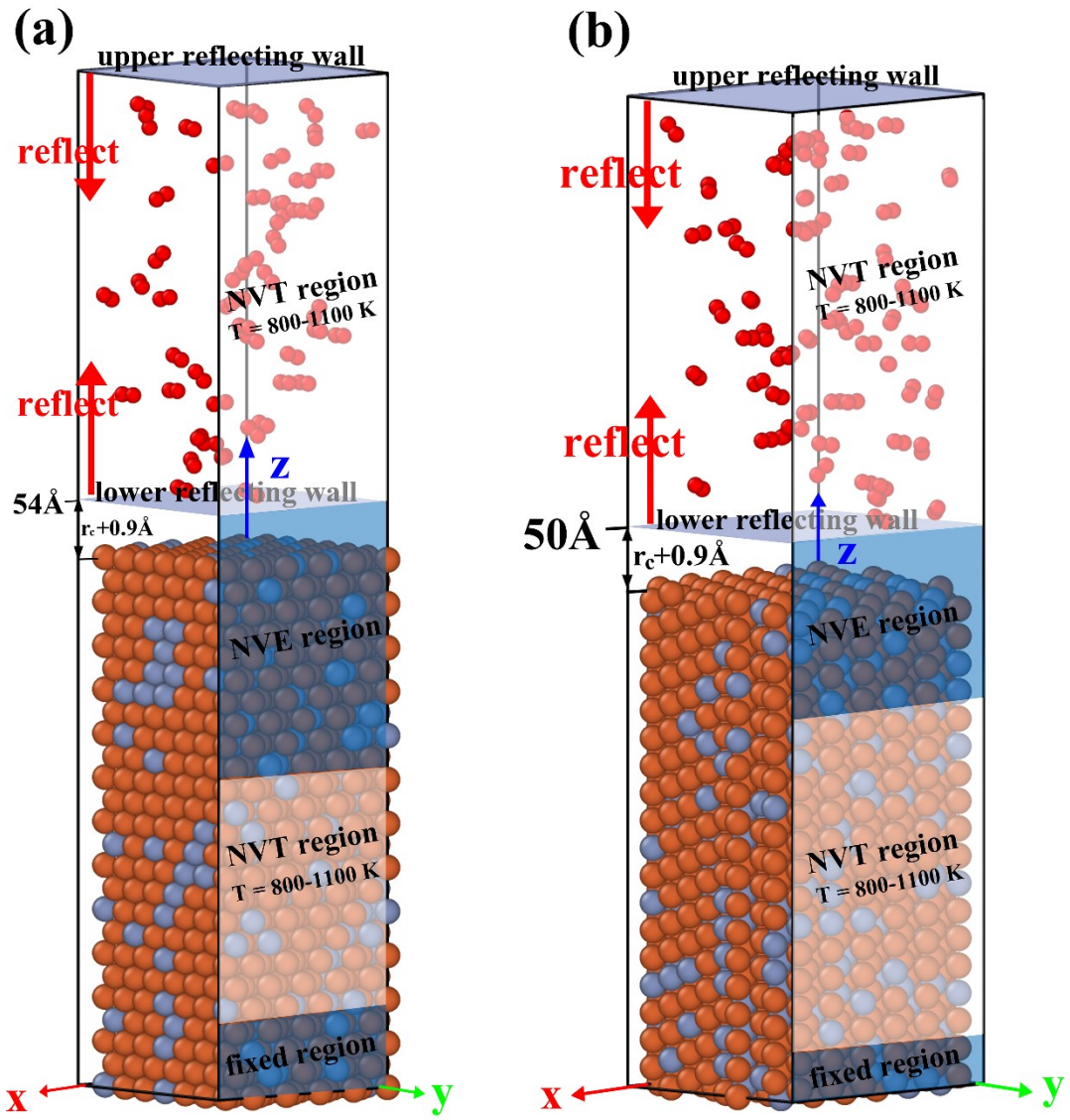

Fig. S1 MD models of Fe-Cr alloy surface with O_2 molecular layers (a) (110) surface (b) (111) surface

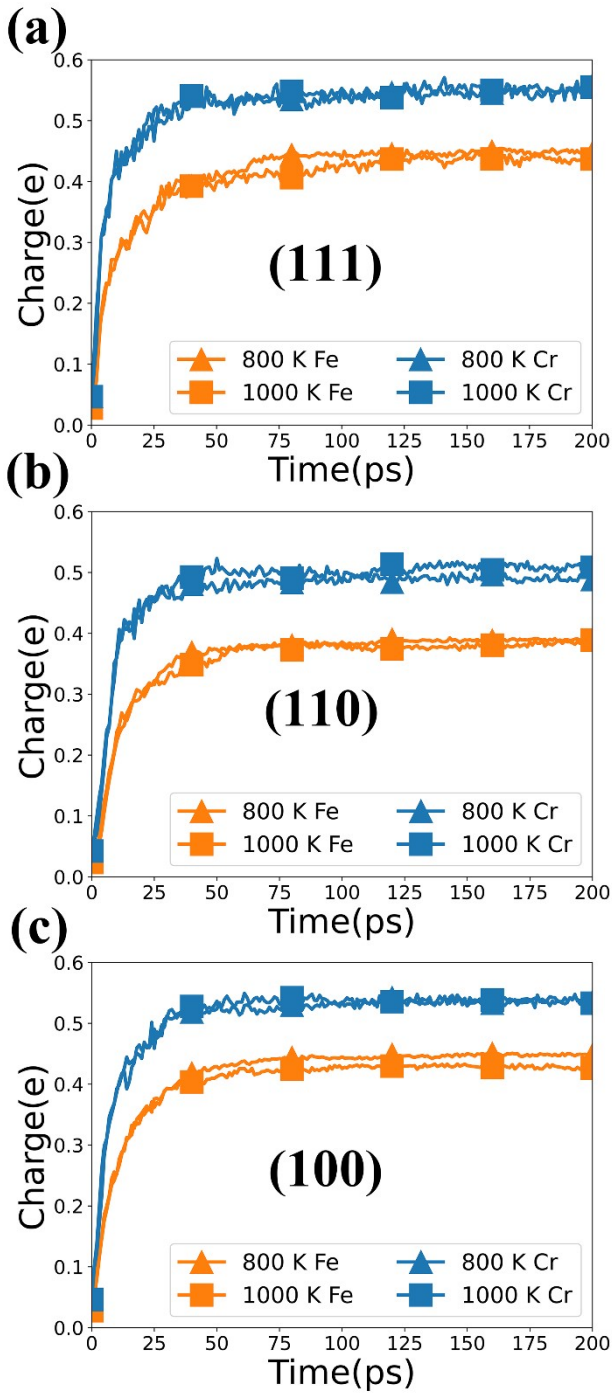

Fig. S2 Average charge variation of Fe and Cr atoms versus time in three types of surfaces at 800 K, 1000 K and high O_2 concentration

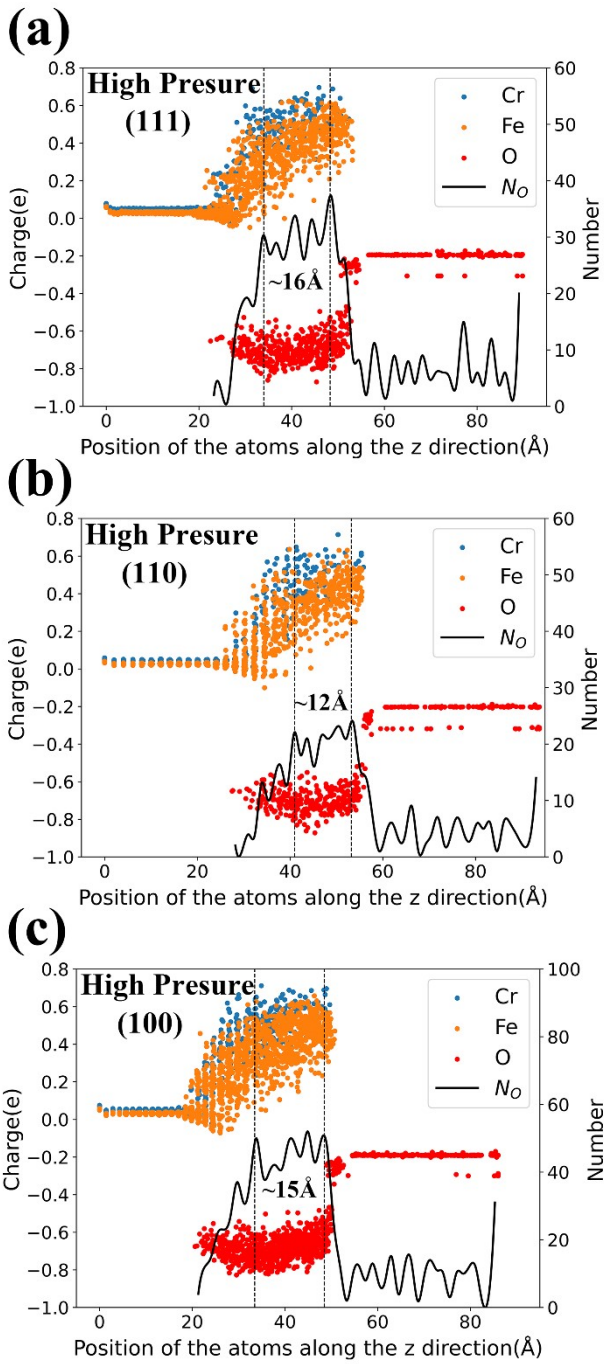

Fig. S3 Left axis: Atomic charge distribution in Z direction of three types of surfaces at 200 ps, T=800 K and high O_2 concentration. Right axis: Corresponding number distribution of O atoms in Z direction

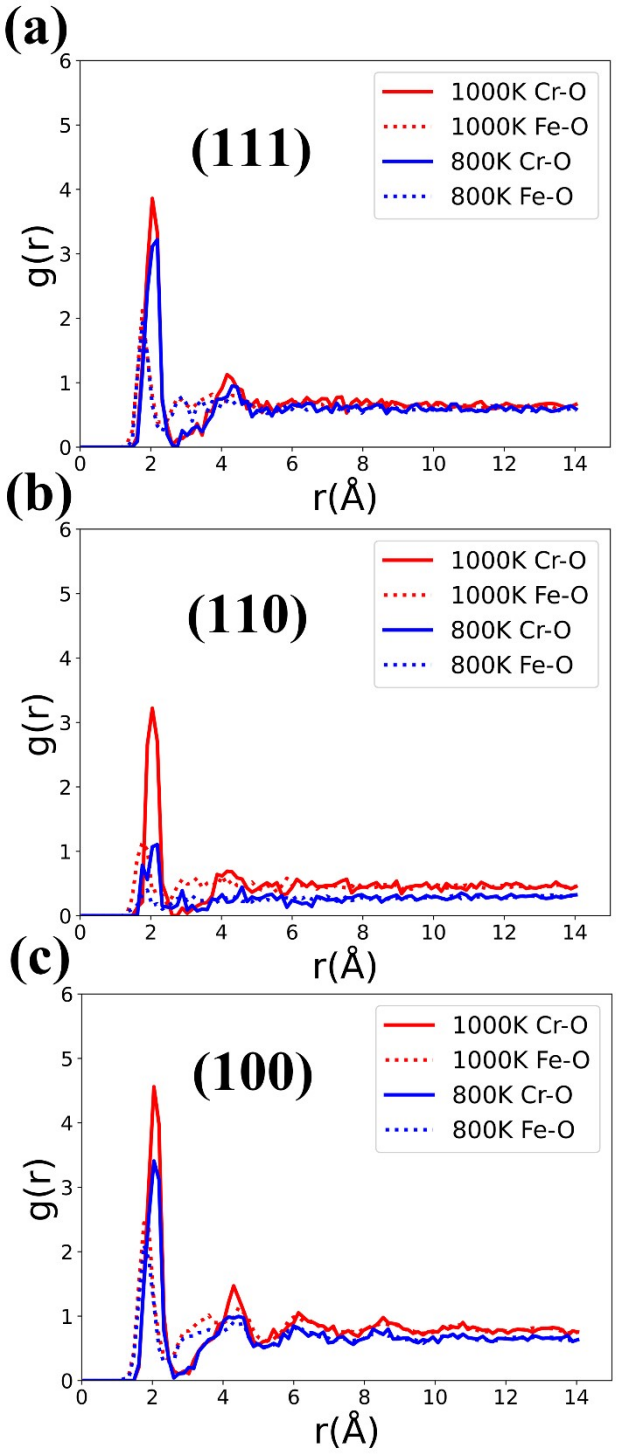

Fig. S4 RDF of Fe-O and Cr-O bonds in three types of surfaces at 800 K, 1000 K and low O_2 concentration