## **Electronic Supplementary Material**

## Experimentally validated atomistic simulation of the effect of relevant grinding parameters on work piece topography, internal stresses, and microstructure

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**Fig. S1** Time series of the topographic distributions for representative molecular dynamics (MD) systems ground at 12 nm infeed depth. This figure corresponds to the data shown in Fig. 4 of the main manuscript, but in a transposed fashion to show an entire time series for one system per panel. All peaks have been centered about their maximum value.

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Fig. S2 Initial topographies of the simulated ferrite and steel systems (top) and the respective topographic distributions and power spectral densities of the surfaces (bottom), evaluated parallel (almost horizontal, dashed) and normal (almost vertical, solid) to the selected grinding direction.



**Fig. S3** Time development of the power spectral densities (PSD) for representative MD surfaces ground at 12 nm infeed depth. The left column shows the PSD parallel to the grinding direction, the right one normal to the grinding direction, showing clear evidence of the evolving anisotropy caused by the unidirectional grinding process.



**Fig. S4** Representative final topographies of experimentally ground work piece surfaces, after (top to bottom) 30, 60, 90, and 150 work pieces without dressing. The right column shows the corresponding power spectral densities normal (blue) and parallel (red) to the grinding direction.