Supplementary materials

S.1 Distance heatmaps for noisy measured spectra

Additional distance heatmaps for measured spectra with additive noise are presented in Figures S 1, S 2, and S 3. In comparison to the noise-free spectra (in the main article), the distance contrast worsens with the growing noise amplitude. Only the Siamese metric can handle the highest studied noise level.

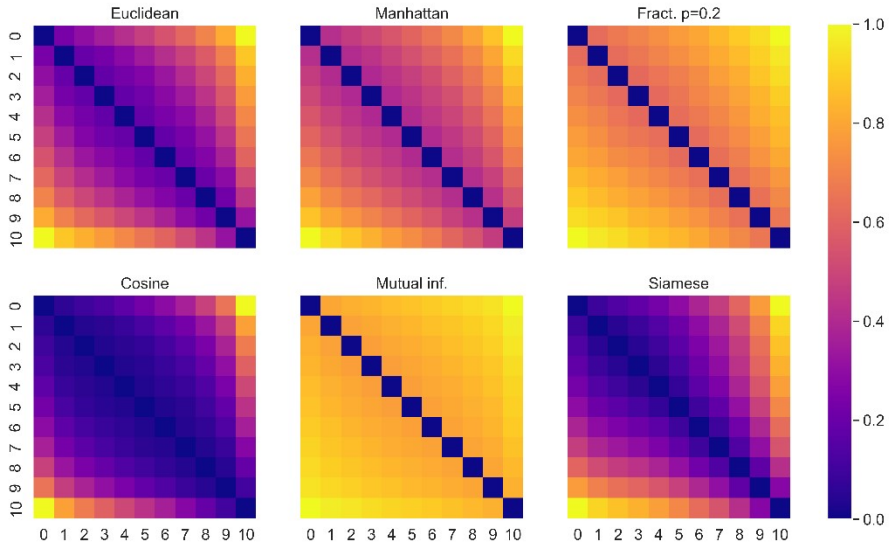

Figure S 1. Distance heatmaps for (sample mean) noise-augmented spectra from the Fe-Co measured dataset. Each metric is normalized by a max value. Noise is from the distribution N(0, 0.01).

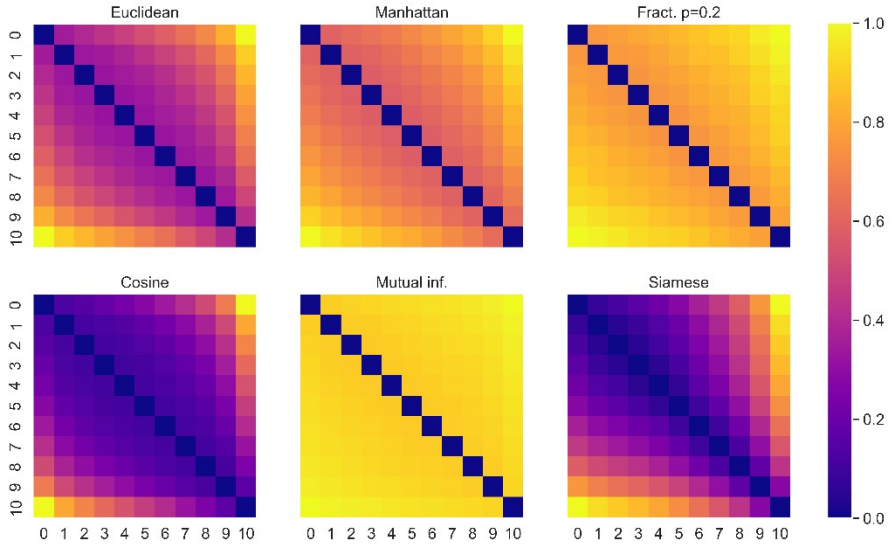

Figure S 2 Distance heatmaps for (sample mean) noise-augmented spectra from the Fe-Co measured dataset. Each metric is normalized by a max value. Noise is from the distribution N(0, 0.02).

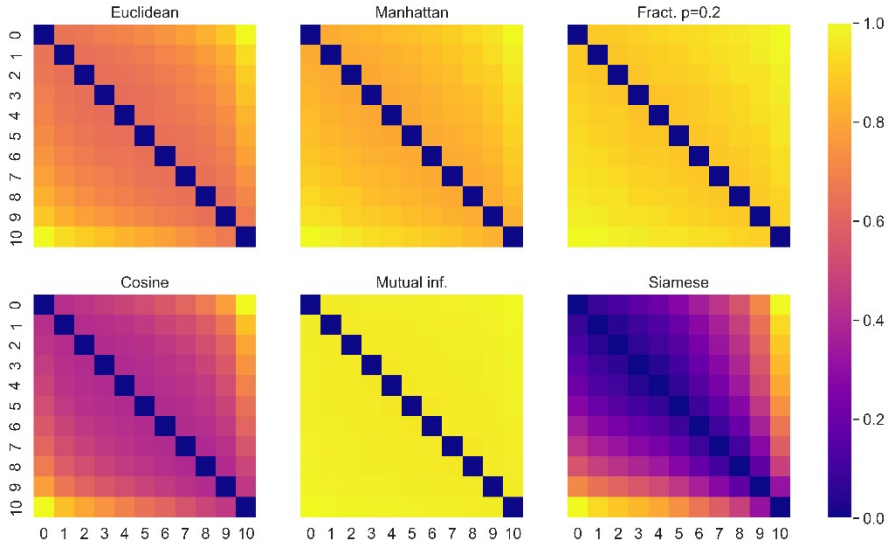

Figure S 3 Distance heatmaps for (sample mean) noise-augmented spectra from the Fe-Co measured dataset. Each metric is normalized by a max value. Noise is from the distribution N(0, 0.05).

S.2 Distance heatmaps for noisy simulated spectra

Here, we show additional distance heatmaps for generated spectra with additive noise (see figures S 4, S 5, and S 6). In comparison to the noise-free spectra (in the main article), the distance contrast worsens with the growing noise amplitude. The numerical artifacts in the Siamese metric with follow from the fact that the model was trained solely on measured data.

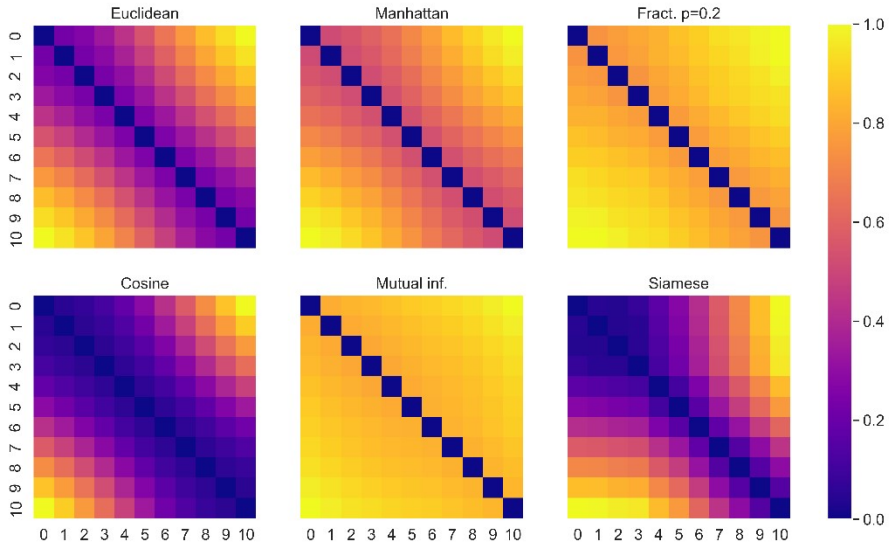

Figure S 4 Distance heatmaps for noise-augmented spectra from the Fe-Co simulated dataset. Each metric is normalized by a max value. Noise is from the distribution N(0, 0.01).

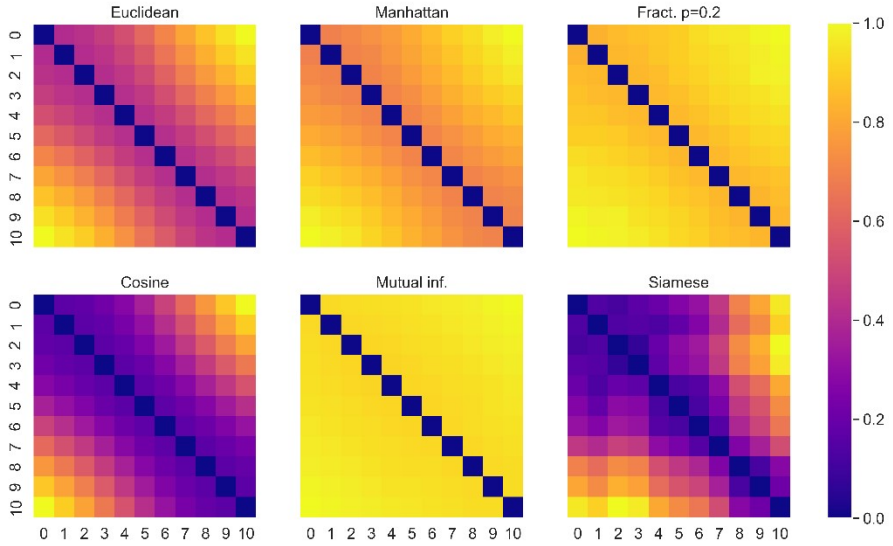

Figure S 5 Distance heatmaps for noise-augmented spectra from the Fe-Co simulated dataset. Each metric is normalized by a max value. Noise is from the distribution N(0, 0.02).

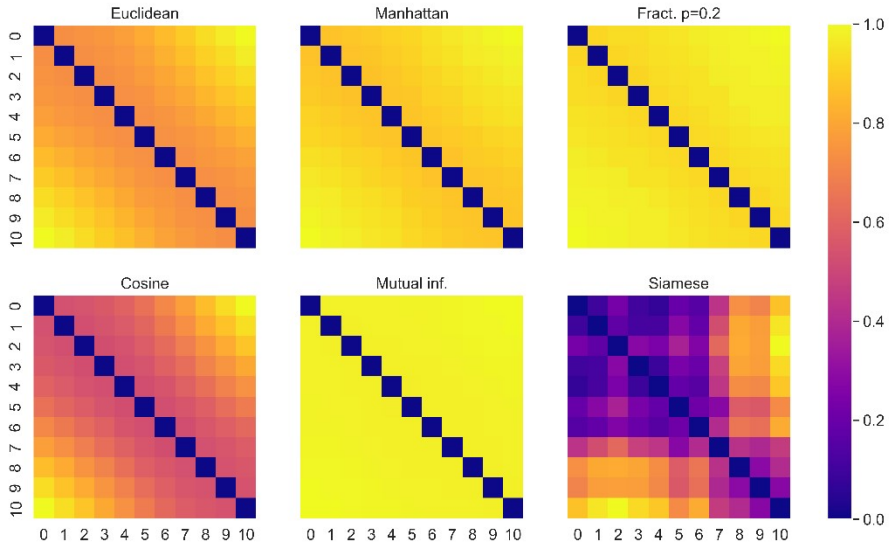

Figure S 6 Distance heatmaps for noise-augmented spectra from the Fe-Co simulated dataset. Each metric is normalized by a max value. Noise is from the distribution N(0, 0.05).

S.3 Signal intensity dependence extra figures

Here, we show additional figures for the varying signal intensities (obtained by using different laser energies).

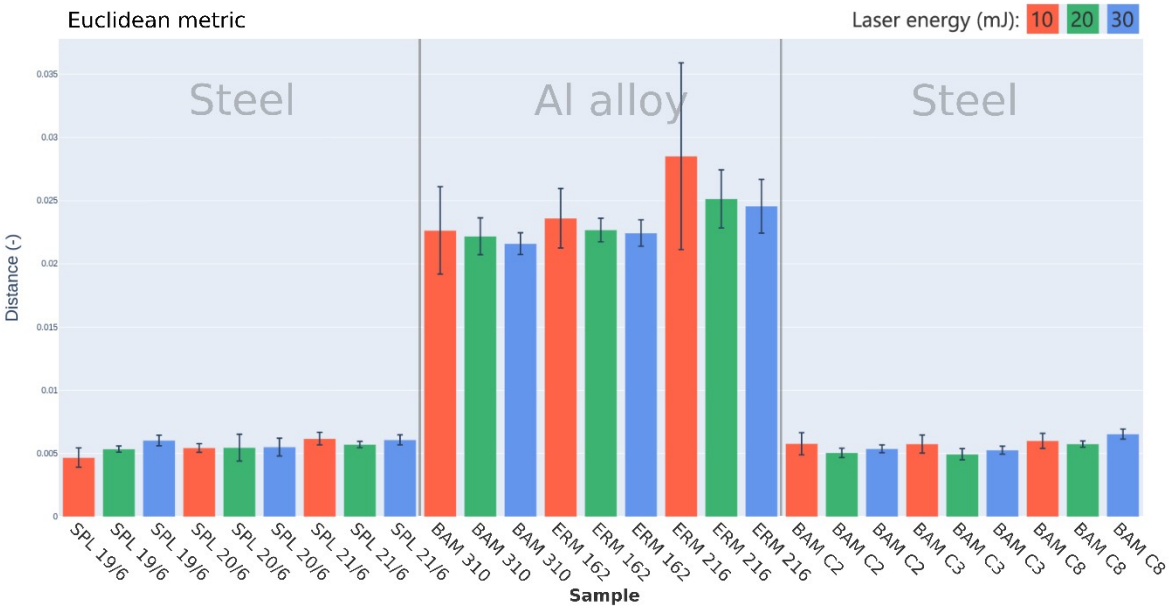

Figure S 7 Max-normalized spectra: Euclidean distances between the reference spectrum (steel sample, laser energy 10 mJ) and corresponding spectra from the Fe & Al dataset.

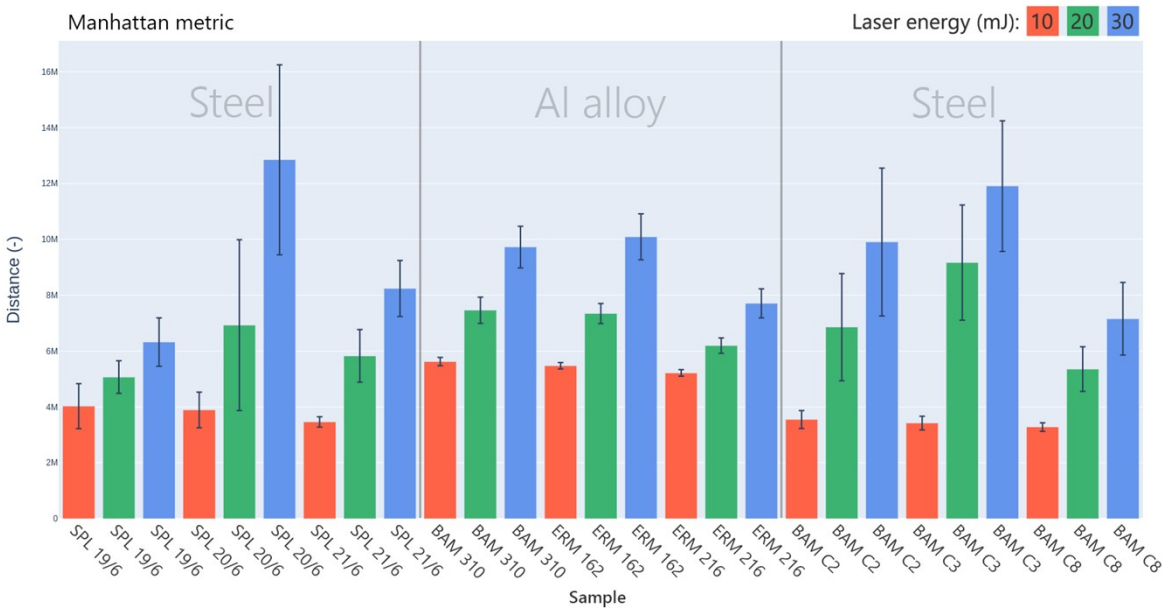

Figure S 8. Manhattan distances between the reference spectrum (steel sample, laser energy 10 mJ) and corresponding spectra from the Fe & Al dataset.

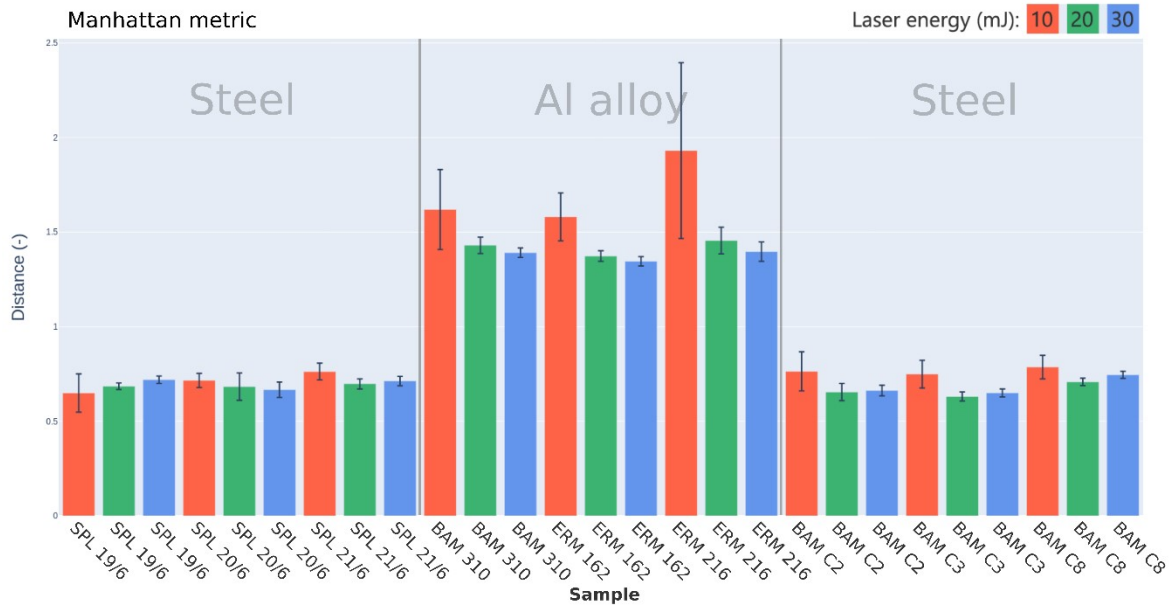

Figure S 9. Max-normalized spectra: Manhattan distances between the reference spectrum (steel sample, laser energy 10 mJ) and corresponding spectra from the Fe & Al dataset.

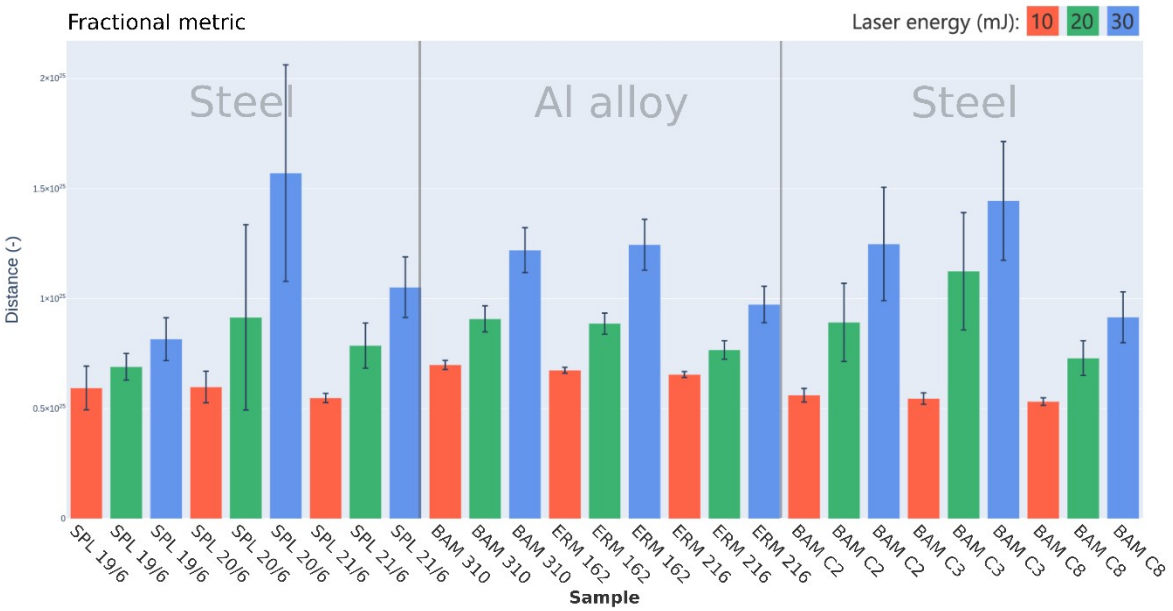

Figure S 10. Fractional distances between the reference spectrum (steel sample, laser energy 10 mJ) and corresponding spectra from the Fe & Al dataset.

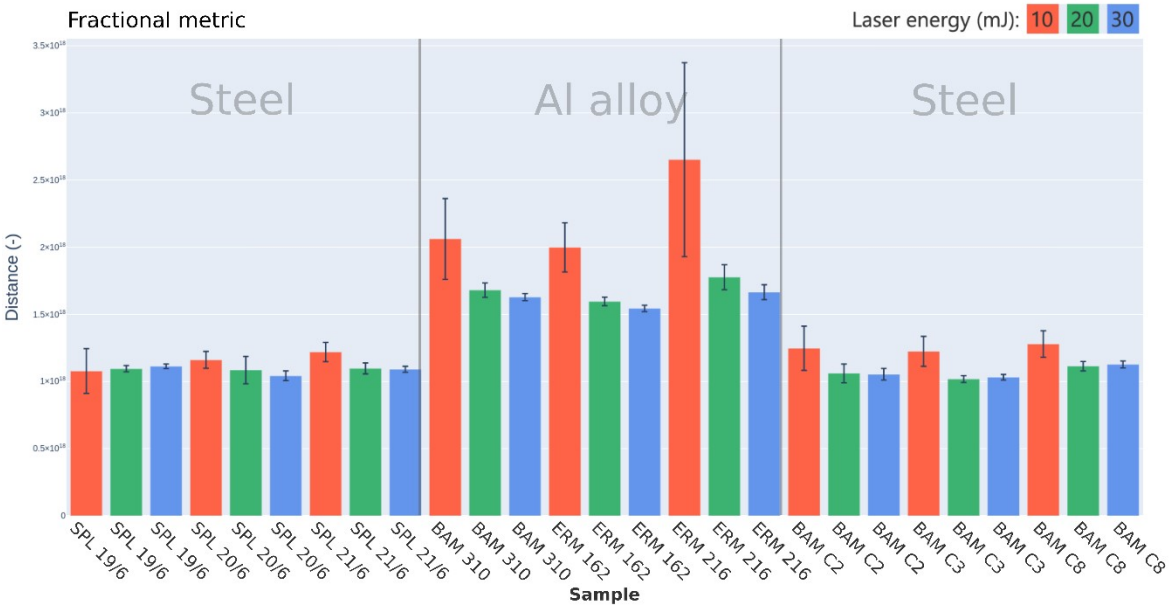

Figure S 11. Max-normalized spectra: fractional distances between the reference spectrum (steel sample, laser energy 10 mJ) and corresponding spectra from the Fe & Al dataset.