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Continuous Wavelet Transforms for Measuring Roughness of Nanoscale Interfaces

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An important observable characteristic of a buried interface between layers or surface of a film is the *interface roughness* (IR). Here we present a *continuous wavelet transform* (CWT) description of the interface roughness as an alternative to the traditional *root-mean-square* (RMS) roughness.

The IR determines the electron transport properties along the interface, and so interfaces can be designed for specific desired outcomes [1]. To be able to relate IR to electron transport properties a detailed description that extracts the salient features of the interface morphology yet provides a condensed interpretation of the IR is necessary. The ideal IR description should allow comparison between IR measurements using any method, should not be sensitive to changes in *signal to noise ratio* (SNR), and should be able to extract sudden peaks in the interface.

To obtain the traditional RMS IR a least-squares minimized plane is fitted to the interface, and the average distance from the fit to the data points is calculated. This approach provides a single value that makes comparing two interfaces convenient. However, reducing the data from a three-dimensional surface to a single value loses data which eliminates important information on the interface properties. Further, RMS measurements are sensitive to SNR [2]. Fig 1 shows computer simulated interfaces that have the exact same RMS value, even though they are visually different. The first interface is a smooth summation of two sinusoids in orthogonal directions, while the second is an evenly spaced grid of periodic Gaussian spikes that are narrow and tall. These two interfaces would have radically different electron transport properties, though the RMS values cannot distinguish any difference between the two.

The one-dimensional CWT for interfaces offers an alternative IR description [3]. CWTs convolve a line of the interface with a one-dimensional spatially finite and amplitude bounded oscillatory signal called a wavelet. The wavelet is spatially modified by a scale factor repetitively, and each convolution generates a plane of spatial information versus scale factor information [4]. The process is reproduced line-by-line over the entire interface. To further simplify the CWT results for ease of viewing, the spatial axes can be averaged out for each scale factor, leaving a line plot of scale versus wavelet content, referred to as the *average wavelet transform* (AWT). Alternatively, the maximum value for each scale factor can be plotted, referred to as the *maximum wavelet transform* (MWT). One popular wavelet choice is the Morse wavelet, with parameters γ and β that affect the shape and number of oscillations in the wavelet [5]. This work makes use of the Morse wavelet with the parameter set $(\gamma, \beta) = (9, 3)$. When using the Morse wavelet with these parameters, the scale factor is a close approximation to the frequency of variations.

The AWT analysis procedure was applied to the interfaces in Fig 1a and Fig 1b, and results are shown in Fig 1c. The plot correctly shows that Fig 1a has a period of 500 samples, which is the period of the sinusoidal interface. The major contribution from Fig 1b is measured at a period of roughly 150 samples, which is the grid spacing, while the other lesser contributions are due to secondary frequencies of a CWT of an individual Gaussian function. Using the AWT approach the differences in IR are clearly observable even when the RMS values are identical.

Sparse features in an interface can also be detected using CWTs. Shot noise was added to the sinusoidal interface from Fig 1a, resulting in the interface shown in Fig 2a. The Fig 2b interface differs from Fig 2a only by a narrow low-amplitude Gaussian feature. Note that the RMS values of these two interfaces are nearly identical. The plot in Fig 2c is the MWT of both interfaces. The contribution to the plot that has a period of 200 samples and less represents the noise, and the peak at a period of 500 samples corresponds to the sinusoidal interface buried in the noise. The only difference between the two interfaces in the results is a cluster of peaks centered at 30 samples, which is due to the presence of the single Gaussian peak in Fig 2b. Using the MWT, the peak is clearly detected amongst both the strong noise as well as the sinusoidal interface. A single peak in an interface can have a significant effect on the interface properties, such as leakage current in an electronic device. Therefore detecting such a feature is a useful characteristic of the proposed CWT description of IR.

The CWT method of measuring IR has benefits that the RMS method does not. With the CWT method, recurring frequencies can be identified over the entire interface by using an AWT. Noise in the data can be distinguished from the interface with ease, as the CWT method is highly resistant to poor SNR. Finally, sparse features of an interface can be detected and located by using the MWT.

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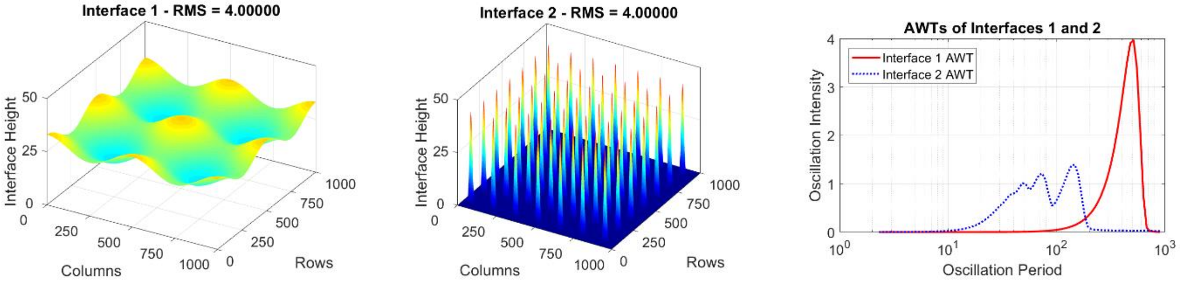

Figure 1. Simulation of two interfaces that are different but have the same RMS value. Results are of the AWT of the two interfaces with frequency plotted on the horizontal axis on a logarithmic scale.

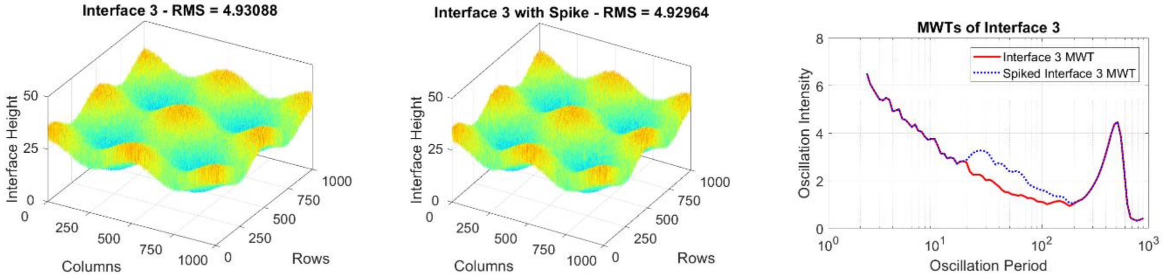

Figure 2. Simulation of a noisy sinusoidal interface, where the only difference between interfaces is a thin Gaussian peak at (row, column) = (300, 700). Results are of the MWT of both interfaces.

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