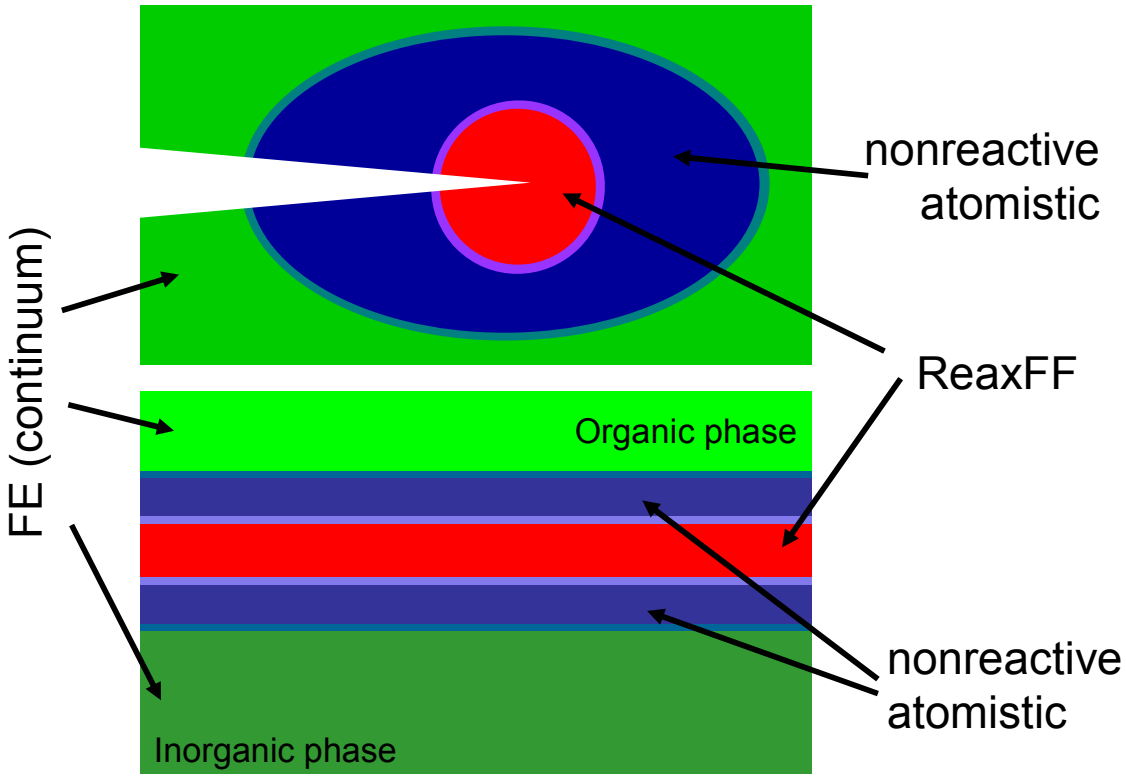
Hybrid Hamiltonians



$$H_{tot} = H_{\text{ReaxFF}} + H_{\text{EAM}} + H_{\text{ReaxFF-EAM}} + \ldots$$

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Hybrid Hamiltonians

$$H_{tot} = H_{\text{ReaxFF}} + H_{\text{EAM}} + H_{\text{ReaxFF-EAM}}$$

$$H_{\text{ReaxFF-EAM}} = w_{\text{ReaxFF}}(x) H_{\text{ReaxFF}} + (1 - w_{\text{ReaxFF}}) H_{\text{EAM}}$$

w_{ReaxFF} is the weight of the reactive force field in the handshaking region.

$$F_{\text{ReaxFF-EAM}} = \left(w_{\text{ReaxFF}}(x) F_{\text{ReaxFF}} + (1 - w_{\text{ReaxFF}}) F_{\text{EAM}}\right) - \frac{\partial w_{\text{ReaxFF}}}{\partial x}\left(H_{\text{ReaxFF}} - H_{EAM}\right)$$

0

Slowly varying weights: $\partial w_{\text{ReaxFF}} / \partial x \approx 0$

Or, alternatively, if $H_{\text{ReaxFF}} - H_{EAM} \approx 0$ (i.e., both FFs have same energy landscape)

$$F_{\text{ReaxFF-}EAM} = \left(w_{\text{ReaxFF}}(x) F_{\text{ReaxFF}} + (1 - w_{\text{ReaxFF}}) F_{\text{EAM}}\right)$$

$$F_{\text{hybrid},N} = \sum_{i=1..N} w_i F_i \qquad \sum_i w_i = 1$$

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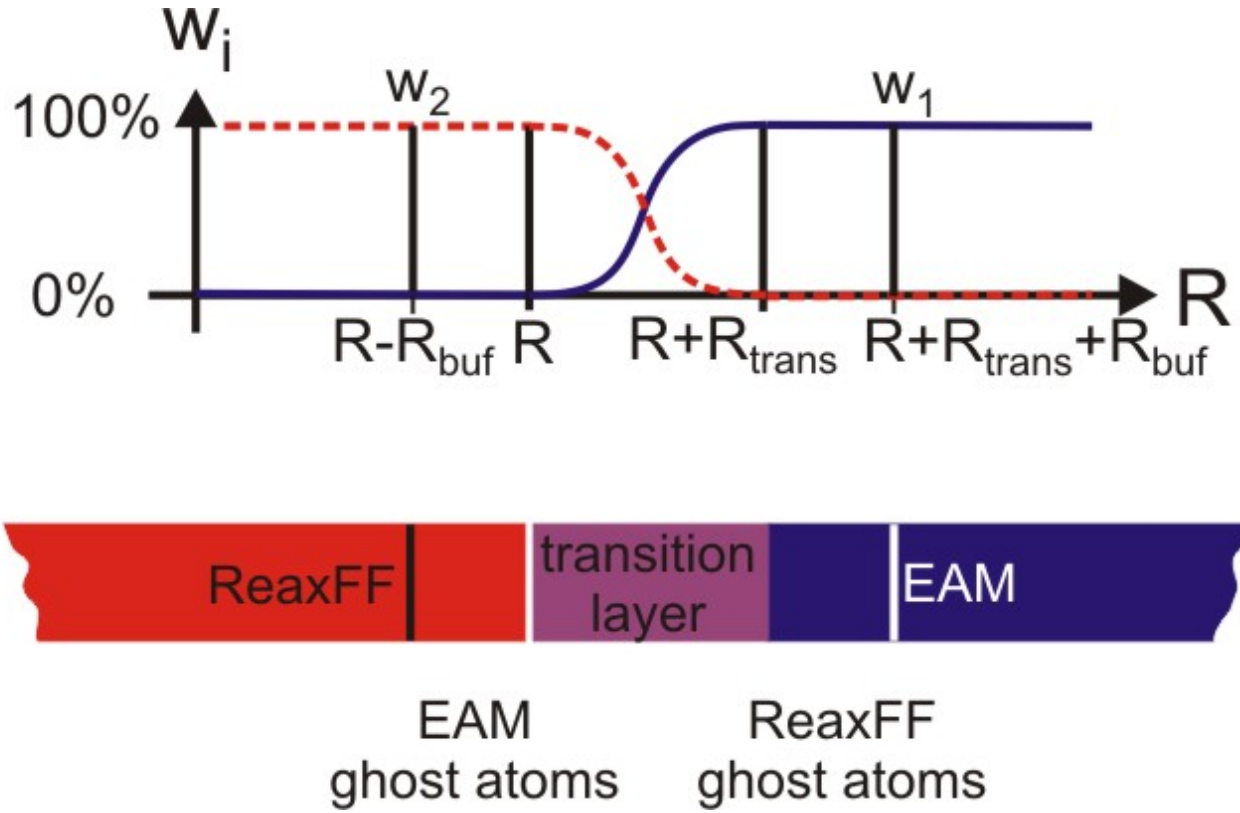
Hybrid Hamiltonians



Rules

1. Handshaking sufficiently far from regions in which methods deviate
2. Slowly varying weights

Both effects help to satisfy simplification

$$F_{\mathrm{ReaxFF}-EAM} = \left(w_{\mathrm{ReaxFF}}(x)F_{\mathrm{ReaxFF}} + (1-w_{\mathrm{ReaxFF}})F_{\mathrm{EAM}}\right)$$

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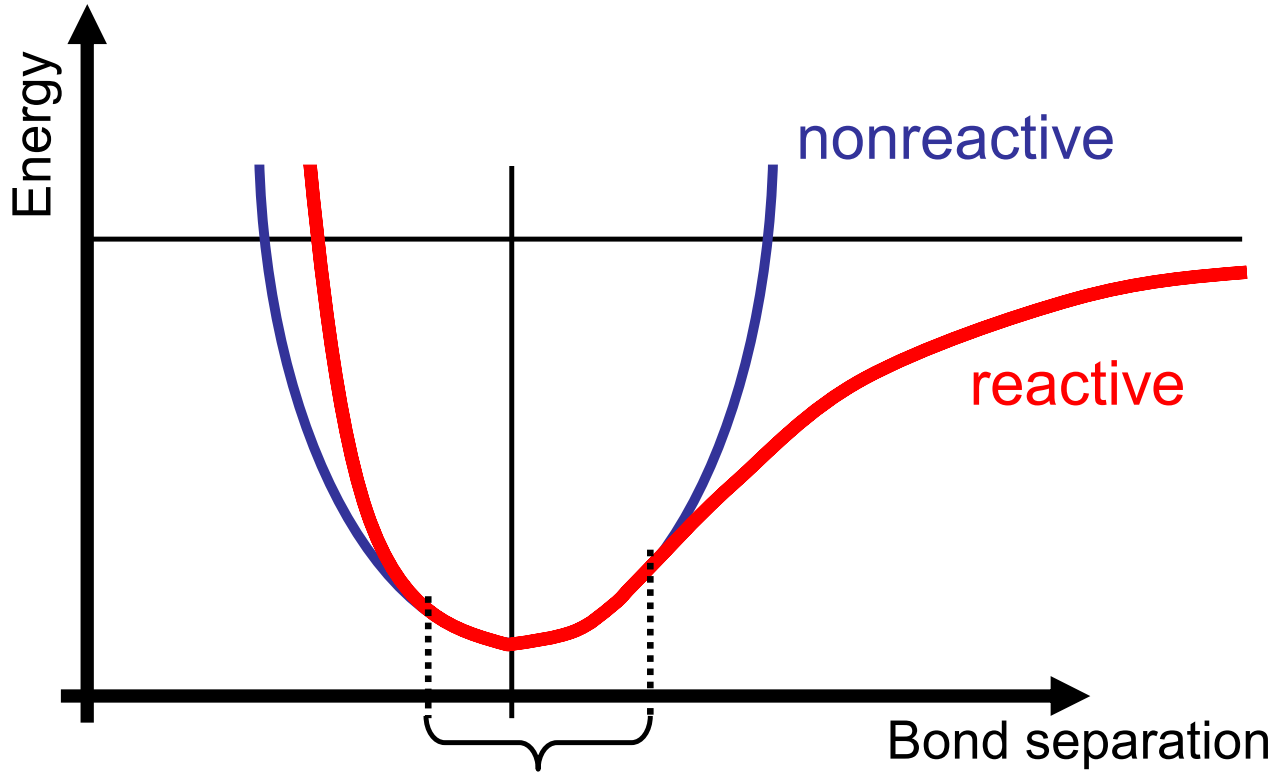
Reactive versus non-reactive potential



reactive≈nonreactive

Handshaking possible

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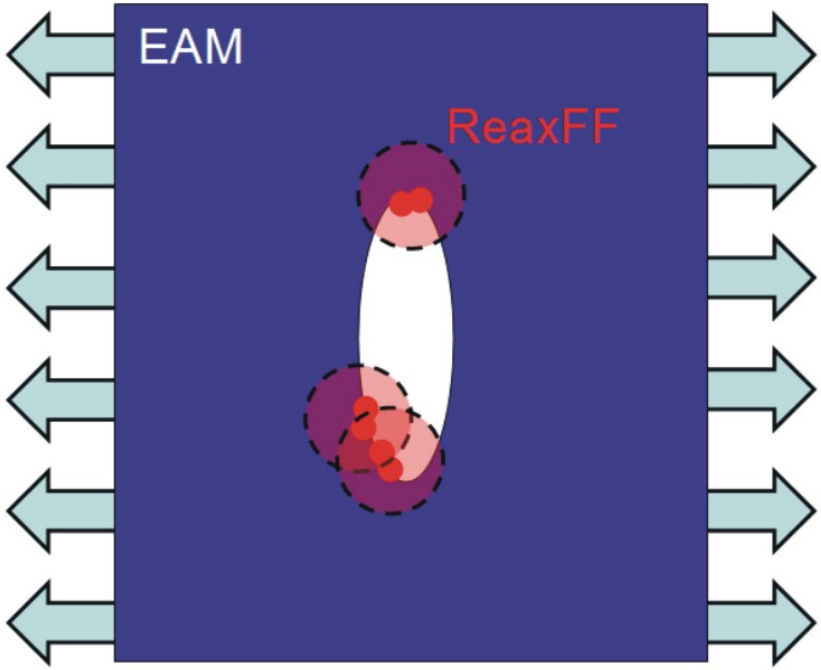
Hybrid Hamiltonians



Schematic showing presence of oxygen molecules inside an elliptical crack in a metal crystal (oxygen molecules are marked by a red color). The oxygen molecules react with metal atoms on the crack surface to form the oxide, and also introduce lattice defects in the bulk metal.

Metal atoms in the vicinity of oxygen atoms and the oxygen atoms themselves can be simulated by a reactive force field, ReaxFF. The bulk metal atoms are simulated using an EAM potential.

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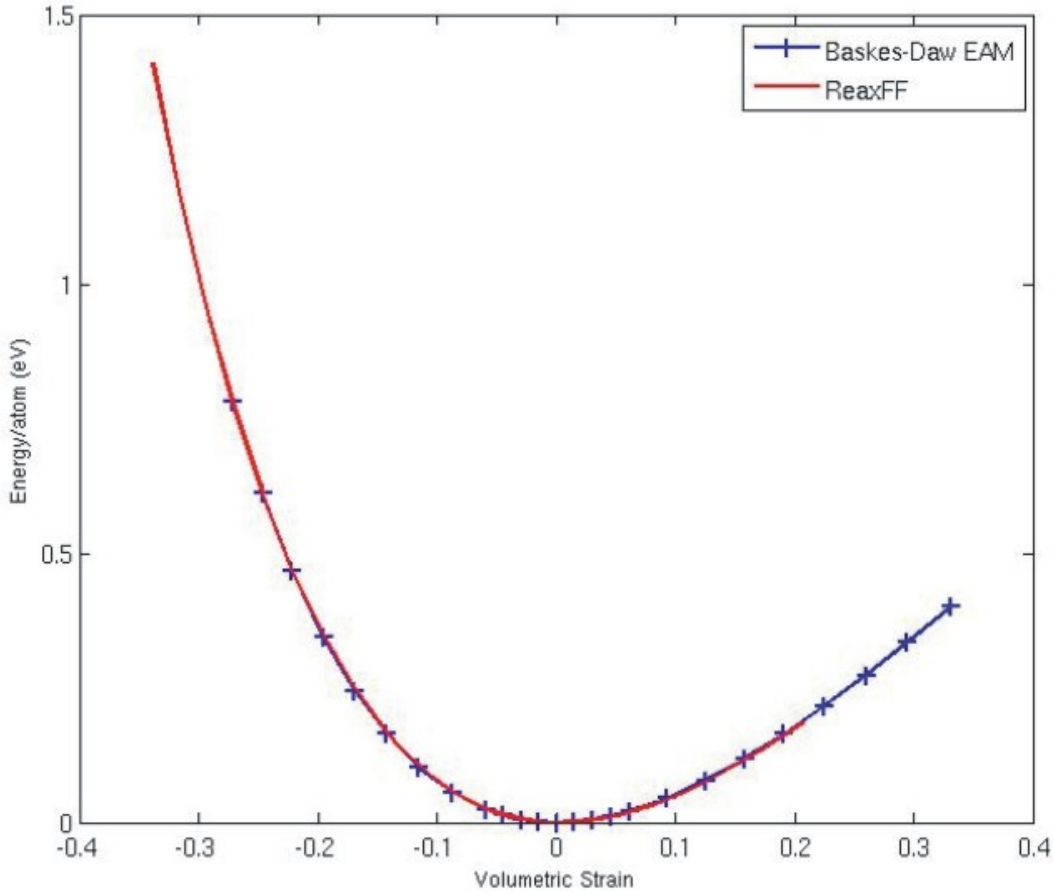
EOS: Comparison EAM-ReaxFF



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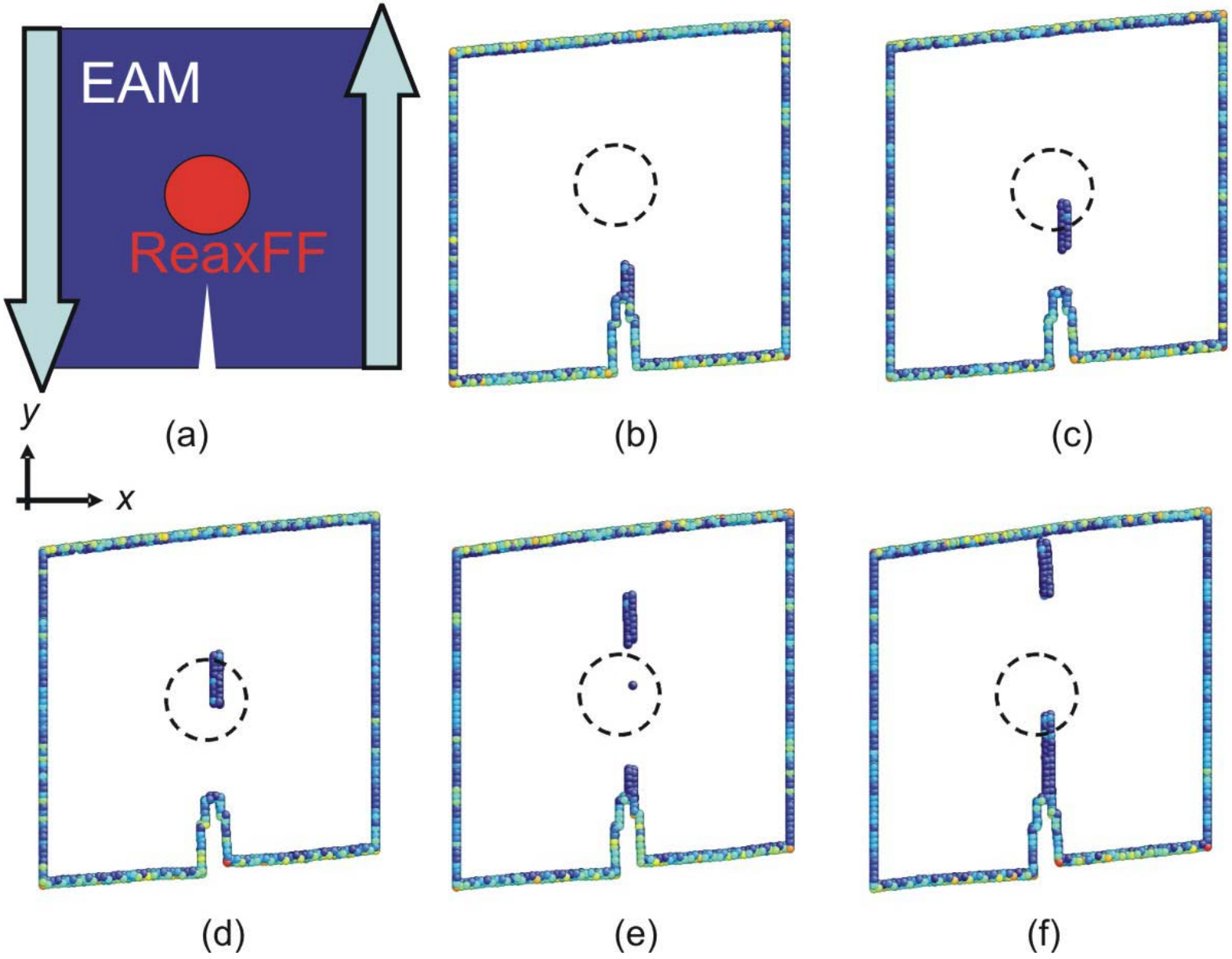
Validation



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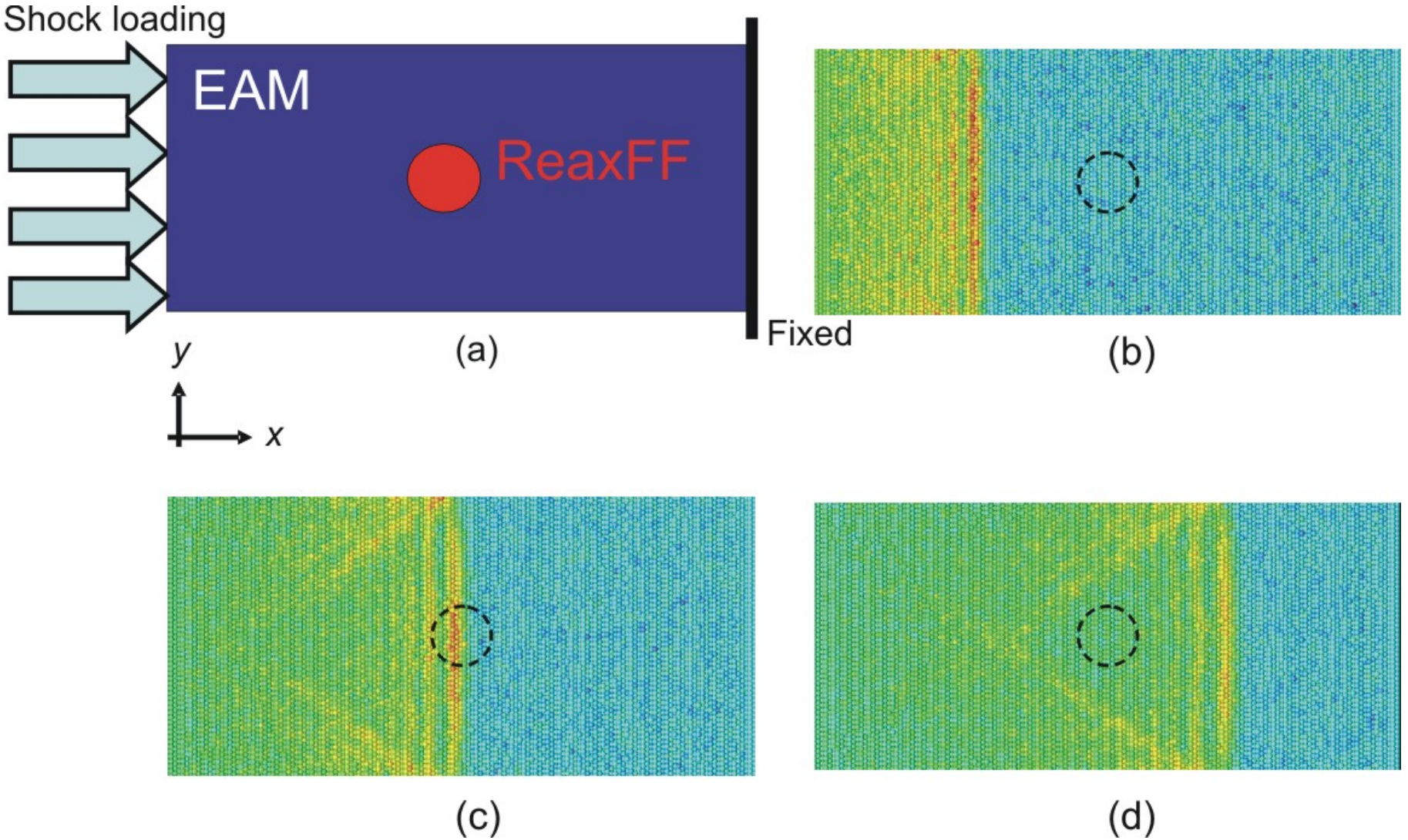
Validation



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