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C2-NEB: THE NUDGED ELASTIC BAND METHOD WITH TWO CLIMBING IMAGES, VALIDATED ON THE NiTi SHAPE-MEMORY MARTENSITIC TRANSFORMATION

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For solid-solid phase transformations in inorganic materials, we developed a nudged-elastic band (NEB) method with two concomitant climbing images (C2-NEB) that can find a transition state in complex energy landscapes, including those with a serpentine minimal energy path. We validate it on the solid-solid phase transformations in Ti and NiTi.

New discoveries often require development of new methods. To address a solid-solid phase transformation on the atomic scale at a finite temperature, one should know the involved terminal stable structures and have a method for controlling atomic motion during the transformation. The nudged elastic band (NEB) method coupled with density-functional theory (DFT) is often used to determine the minimum-energy path (MEP) and the transition states (TS). We broaden the NEB applicability and provide an extension to two climbing images (C2-NEB) method \cite{1,2} that is more stable and reliable for complicated potential-energy landscapes.

For validation, we applied the C2-NEB \cite{1} to the solid-solid phase transformations in NiTi \cite{2,3,4}. We found the minimal energy path with a small potential energy barrier for the martensitic transformation between NiTi austenitic and martensitic phases \cite{3}. Considering a 2-dimensional (2D) example with a twisted MEP having a zigzag near the TS (see Fig.5 in \cite{2}), we demonstrated that C2-NEB is more efficient, because it can find the TS with only 3 images, while C1-NEB \cite{5} can require up to 35 images for convergence to the lowest-energy saddle.

![Fig. 1: Ti α–ω transformation under pressure. Enthalpy (solid line) and excess volume (red dashed line, middle scale) from no-climbing NEB (open circles) and C2-NEB (larger circles) methods. Insets are the structural projections of the supercell along [110] and [001] at enthalpy extrema. Ti atoms on the alternating hcp planes are black and blue.](image-url)
Figs. 1 and 2 in [2] illustrate a 2D potential energy landscape, for which C2-NEB with only 3 images works correctly and finds the TS, while the convergence criteria of C1-NEB with a small number of images will never be satisfied.

Here we apply the C2-NEB code [1] to the α–ω transformation in pure Ti under pressure (Fig. 1). As expected [2], we confirm stability of the C2-NEB code, which is available online [1].

In the C2-NEB method [1,2], at each optimization step, the highest-enthalpy image (HEI) is found. If both neighbors of the HEI are movable (i.e., they are not the fixed terminal points), then they climb, approaching the HEI, which is nudged to them. C2-NEB method [2] can be coupled with any DFT or classical molecular dynamics code, capable of computing structural enthalpies and atomic forces. Our code [1] is combined with VASP [6], which provides the atomic forces and the total enthalpy (TOTEN variable) for each image. Implemented to replace the NEB subroutine in VASP, our C2-NEB open-source code is available for download [1].

Martensitic transformation in the NiTi shape memory alloy is addressed in refs. [2,3,4]. Pure Ti is one of the most used structural metals. Here we use C2-NEB to locate two enthalpy maxima for the Ti α–ω (TAO-1) transformation [9], see Fig. 1. To correct the well-known systematic DFT error arising from over-binding of d-electrons, we use DFT+U method [7] with (U-J)=2.2 eV, which provides the α–ω equilibrium coexistence pressure of 2 GPa [8]. For faster convergence, first we obtain the whole trajectory without climbing [5]. Interestingly, Ti α–ω transformation [9] has an intermediate minimum (Fig. 1): this is a lower-density metastable structure, which can be stabilized by negative pressures; it has the maximal excess volume ∆V=V(x)–V(0)+x[V(0)–V(1)], where the rescaled NEB path coordinate x changes from 0 (α) to 1 (ω). Then, we separately address each local maximum: we use two images on both sides of a maximum as the terminal points, add 3 images between them, and use C2-NEB to converge those 3 images to the saddle point (larger grey circles in Fig. 1); they converge to the same enthalpy within the DFT error [<0.5 meV/atom], while the central image always remains slightly [−0.1 meV/atom] higher in enthalpy than both climbing images. As expected [2], convergence of the C2-NEB code [1] with only 3 images is stable regardless of any possible zigzags of the MEP.

In summary, we find that the C2-NEB algorithm [1,2] is very useful, especially for systems with a serpentine MEP or unknown behavior of the NEB trajectory near the TS. We validated it on the martensitic transformations in NiTi shape-memory alloy [2,3,4] and in pure titanium under pressure. Our C2-NEB implementation is available as an open-source code [1].

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References