Full length article

On the atomic structure of the β″ precipitate by density functional theory

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ABSTRACT

The substitution of elements into the β″ precipitate in the 6xxx-series of aluminium alloys is an interface sensitive problem. The strain caused by the misfit between the precipitate and the matrix interacts with the size misfit of solute substitutions. The full cross-section of the β″ precipitate and interface was simultaneously studied without the influence of periodic images by applying rigid boundary conditions in a cluster-based model that contained two regions, one fixed and one relaxed. An optimised geometry of the fixed region allows partially occupied atomic columns which enable a more precise description of the various precipitate configurations. A subtle shift in the atomic columns occurred during relaxation from the initial atomic positions in the β″ precipitate, which breaks the notion of a 4-fold symmetry of the β″ eyes. The underlying C2/m symmetry was intact through this shift. The methodology was applied to calculate the relative formation enthalpy of substituting lithium and copper at different atomic sites and benchmarked against previously published density functional theory and transmission electron microscopy studies. The results correspond well with expectations based on the experimental studies available.

1. Introduction

Precipitation strengthening is crucial for achieving optimal mechanical properties in age-hardenable Al alloys. For the 6xxx-series of Al alloys, where Mg and Si are the main alloying elements, the β″ precipitate is the main hardening phase at peak hardness. The precipitation sequence in the 6xxx-series of Al alloys is generally reported as [1–7],

SSSS → Mg/Si clusters → Guinier−Preston (GP) Zones →

→ β″ → β′, U2, U1, B′ → β, Si,

where SSSS is the super-saturated solid solution, β′, U2, U1 and B′ are metastable precipitates and β (Mg₂Si) is the equilibrium phase. Adding additional elements to the alloy can result in different precipitation sequences by stimulating the formation of other precipitate phases [7,8] or, for small additions, elements can be incorporated into the β″ at the various atomic sites. Most elements that can be substituted into the β″ unit cell, e.g. Li [9], Ni [7] and Cu [10–12], do so at preferred atomic sites. In some cases, the inclusion of other elements, such as Ge [13], leads to changes in the atomic arrangement of the β″. Although alterations of the atomic arrangement of the β″ are reported, the C2/m symmetry of the β″ is intact in the β_2'' and β_3'' [13].

A recent investigation of the strain field of the β″ precipitate [14] demonstrated how both the chemical and elastic contributions to the strain field can be accurately described using density functional theory (DFT) without the influence of periodic images. This motivated further application of the methodology to investigate the internal structure of a precipitate embedded in the matrix in addition to the difference in the formation enthalpy of different substitutions in the β″ precipitate.

In this work, the methodology presented in the article by Frafjord et al. [14] is refined and utilised to study the details of the internal structure of β″. DFT is applied to calculate the differences in formation enthalpy of Li and Cu substitutions in the β″ precipitate. The results presented are compared to the investigations by Mørtsell et al. [9] and Saito et al. [11] for Li and Cu substitutions, respectively. The advantages of the methodology presented here are highlighted. The aim of this study is to emphasise the difference in the atomic sites of the β″ precipitate and motivate the use of the methodology applying rigid boundary conditions (RBC) in future studies on formation enthalpy of different elements in embedded precipitates.

2. Method and model

All DFT calculations in this work are performed by using the Vienna Ab Initio Simulation Package (VASP) [15,16]. The generalised gradient

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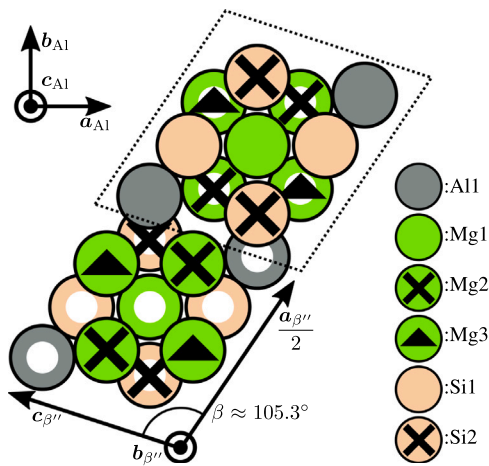*E-mail address:* Jonas.Frafjord@ntnu.no (J. Frafjord).

Fig. 1. Atomic model of the β'' precipitate. The unit cell consists of two formula units called eyes, one of which is marked by a dotted rhomboid. The white circle in some of the atoms indicates that they are in a lower plane than the others. a_{Al}, b_{Al} and c_{Al} are the lattice vectors in Al, while $a_{\beta''}$, $b_{\beta''}$ and $c_{\beta''}$ are the lattice vectors in the β'' precipitate.

Fig. 2. A schematic illustration of the cross-section model of the β'' precipitate, which is relaxed to minimise forces. The inner part is relaxable atoms consisting of the precipitate, coloured in blue, surrounded by the cylindrical shell of Al, coloured in grey. The outer region, coloured in purple, is Al atoms that are held fixed during relaxation. Δ and δ are the width of the fixed and relaxed Al region, respectively. $\hat{a}_{Al}$, $\hat{b}_{Al}$ and $\hat{c}_{Al}$ are the unit vector directions in Al, while $\hat{a}_{\beta''}$, $\hat{b}_{\beta''}$ and $\hat{c}_{\beta''}$ are the unit vector directions in the β'' precipitate. $\beta \approx 105.3°$ is the angle between $\hat{a}_{\beta''}$ and $\hat{c}_{\beta''}$. The surrounding vacuum is represented by the white colour. The model is periodic in the $\hat{c}_{Al}$ direction.

approximation by Perdew–Burke–Ernzerhof [17] is the applied functional. A gamma sampling with maximum 0.18 Å^{-1} separation between k-points is used to model the Brillouin zone and a 400 eV plane-wave energy cut-off is applied. Bulk calculations of aluminium and the β'' precipitate were done, and the Al lattice constant was found to be 4.046 Å.

The β'' precipitate unit cell is illustrated in Fig. 1, where the different atomic sites have been marked. The Al sites are often referred to as the Si3/Al sites due to the reported variations in the composition of the β'' [4]. Previous DFT [18] and energy-dispersive X-ray spectroscopy [19] studies concluded that the most energetically favourable composition is $Mg_5Al_2Si_4$. This composition was used as the reference structure in this study, both for simplicity and for the readily available displacement data for atomic positions [14,20].

The atomic model applied in the DFT calculations is similar to the cluster based model presented in a previous publication [14], also using RBC. One important difference is the use of a rhomboid geometry of the fixed region, as illustrated in Fig. 2. The atoms in the outer region are superimposed by a displacement field prior to relaxation and held fixed during the relaxation. The inner region is relaxed by DFT, influenced by the applied strain field of the fixed region. It is assumed that the inner region is sufficiently screened by the outer region, as to be unaffected by the free surface. The width of the inner and outer region are determined to be $\delta > 7$ Å and $\Delta > 6$ Å, respectively, based on cluster-size calculations. These parameters were found to be independent of the size of the precipitate [14], since the chemical contribution of the displacement field is determined mostly on the distance between the interface and the fixed region. The model is periodic along the needle direction, $\hat{c}_{Al}$, with a slab thickness of one (two) unit vector $|c_{Al}| = |b_{\beta''}| = 4.046\ (8.092)$ Å.

The displacement field superimposed on the Al atoms is calculated from linear elasticity theory, by using finite element method (FEM). The details of the FEM calculation are given by Ehlers et al. [20]. The FEM calculations yield an elastic displacement field that is dependent on the aspect ratio of the precipitate and scaled by the actual size of the precipitate. It is assumed that the displacement field in the fixed region is unaffected by the substitution of a few atoms into the precipitate. This data for the elastic displacement field are available in the Zenodo repository [21] and was superimposed to all atoms in the slab before constraining the atoms in the fixed region.

The formation enthalpy of a precipitate cannot be directly calculated with RBC due to the vacuum surrounding the precipitate.
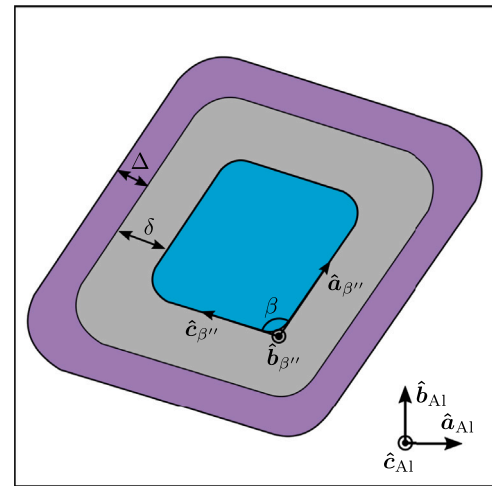
However, the relative formation enthalpy can be calculated since the energy contribution of the surface is canceled out. The relative formation enthalpy of a solute atom, X, substituting an atom, S, at a specific atomic site in the precipitate is calculated by

$$\Delta E_{\beta''}^{S \to X} = (E_{\beta''}^{S \to X} + E_S) - (E_{\beta''} + E_X), \tag{1}$$

where $E_{\beta''}^{S \to X}$ and $E_{\beta''}$ are the energies of the full system with and without the substitution of X into the β'', respectively. The E_S and E_X represent the energy of having the solute S and X in the Al matrix, respectively. The free surface of both full-system models applied in this work is equal, thus the energy contribution is canceled in Eq. (1).

The scanning transmission electron microscopy (STEM) image used in this work was downloaded from the Zenodo repository of Frafjord et al. [21]. It was originally acquired with a double-corrected JEOL ARM-200F microscope, operated at an acceleration voltage of 80 kV. The image was distortion-corrected using Smart Align [22]. A more detailed description of the experimental method can be found in [23].

3. Results & discussion

The relative misfit between the Al lattice vector and the β'' lattice vector was calculated by conducting the DFT relaxation of a $5 \times 5\ \beta''$ precipitate using rhomboid RBC. Details of the misfit calculations can be found in [14]. The misfit value found in this investigation corresponds well with the values previously reported by both experiments and DFT [14,23]. The rhomboid approach has a smaller simulation cell, fewer atoms and a longer minimum distance from the precipitate to the fixed region, for the same precipitate size. The number of relaxable atoms is uniformly distributed around the precipitate, which promotes an unbiased dispersion of the strain energy.

3.1. Placement of atomic columns in the β'' precipitate

Fig. 3 shows the displacement vectors of the atoms in β'' after relaxation, relative to the associated Mg1-site. The initial structure is based on the fcc Al lattice without misfit. The colour of the atoms in Fig. 3 represents the rotation of the atoms around their associated
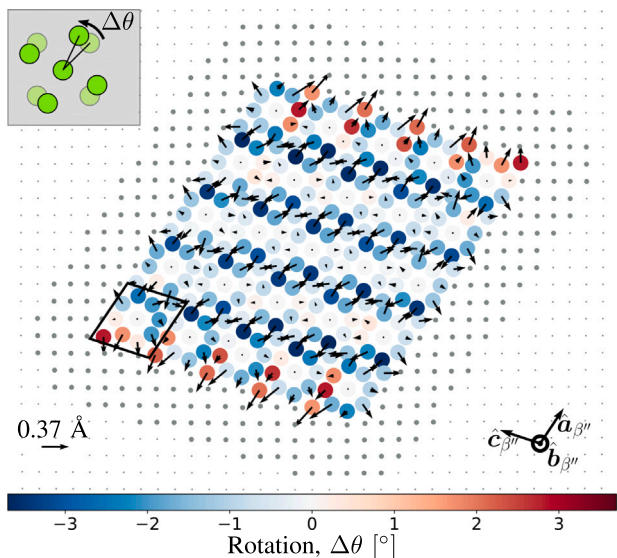
Fig. 3. Atomic positions of a cross-sectional model of a β'' precipitate embedded in Al. The black rhomboid represents one formula unit of the β'' unit cell. Each formula unit contains one Mg1 site, the centre atom, that is assigned with a null vector. The vectors of the other atoms represent the displacement relative to their associated Mg1, after DFT relaxation. The reference vector shows the length of the longest vector. The colour represents the rotation angle, $\Delta\theta$, which is the rotation in the cross-sectional plane of the atomic columns around the centre Mg atom. The positive rotation direction is shown in the grey rectangle.
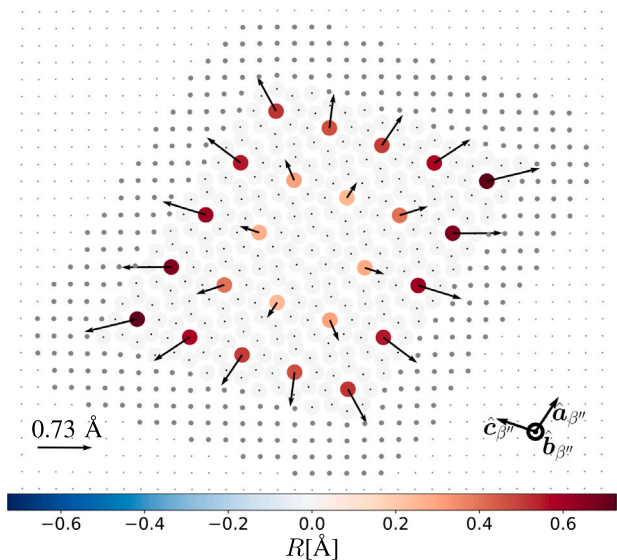

Fig. 4. Atomic positions of a cross-sectional model of a β'' precipitate embedded in Al. The vectors and colour represent the displacement of the atomic columns at the Mg1 sites from the original unrelaxed positions relative to the precipitate main axis, after relaxation by DFT. The vectors are scaled for better visibility, and the label of the reference vector shows the length of the longest vector.

Mg1-site, corresponding to one formula unit as in Fig. 1. The general trend is that the Mg–Si pairs of neighbouring eyes move towards each other, as do the Al atoms. The unit cells expand as a consequence of the expansion of the precipitate, see Fig. 4, where the displacement vectors represent the displacement of the Mg1-sites relative to their initial positions. An expansion of the unit cells and the precipitate is expected since the initial structure was constructed using the zero misfit lattice vectors of β''.

In addition to the expansion, the atomic columns generally rotate a few degrees, $<4°$, in the cross-sectional plane around the central Mg

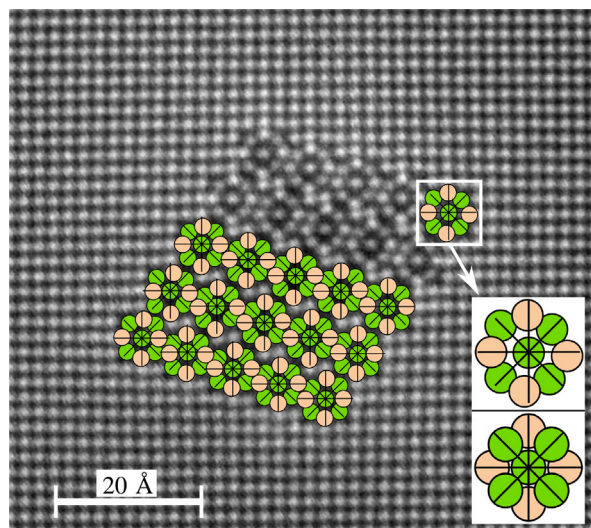**Fig. 5.** A STEM image of a 5 × 5 β'' precipitate, downloaded from the Zenodo repository of Frafjord et al. [21]. The atomic columns are overlaid by hand, where Mg and Si are represented by green and beige circles, respectively. The Al atoms are excluded in the overlay. The upper inset shows an enlarged version of the outlined eye. The lower inset shows a β'' precipitate eye, with zero misfit with respect to the Al fcc lattice.

column. The same displacement is observed for relaxation of both the bulk structure and the β'' cross-sections embedded in the Al lattice. Fig. 5 shows a STEM image of a 5 × 5 β'' precipitate, downloaded from the Zenodo repository of Frafjord et al. [21]. The image has been analysed and overlaid manually by careful placement of the atomic columns. The STEM results confirm that the subtle movement in the atomic columns is observed experimentally and is not an artefact from the numerical method.

The structural perturbation of the atomic columns is symmetric and does not change the inherent C2/m symmetry. The subtle change in the atomic structure of the β'' unit cell is a reminder that the different atomic sites in the β'' unit cell are unique. The emphasis is in contrast to published work which refers to the β'' eyes with 4-fold symmetry [9,11,24] with satellite columns. The displacement and rotation of the atoms relative to the Mg1-site observed in this study break the possibility of a 4-fold symmetry being relevant for β'' precipitates larger than a single eye.

3.2. Advantages of a cluster-based approach

The consequences of the uniqueness of the atomic sites are highlighted when different alloying elements are added to the 6xxx-series of Al alloys. The experimental results in the paper by Mørtsell et al. [9] show that the lithium (Li) atoms occupy the Mg3 sites when the eye is not adjacent to the interface. The DFT calculations conducted in that work indicate that the Mg1 sites should be preferred before the Mg3 sites, contrary to the experimental evidence presented. These calculations were conducted for bulk β'', i.e. without an Al interface. Embedding the precipitate into the Al lattice compresses the bulk β'' and results in an associated internal strain field [23]. Thus, neglecting the interface may lose crucial contributions to the formation enthalpy.

Other observations considering the flavours of the β'' are presented by Saito et al. [11], where Cu is shown to occupy Si3/Al sites near the interface. The challenge of modelling element substitutions in β'' was stressed in this paper, and the emphasis was placed on the relevant strain fields introduced when a β'' is embedded in the Al lattice. The periodic images of a traditional supercell methodology influence the strain field. These issues are circumvented in the methodology used in this work since the RBC should correct for the effect of the strain field.

Table 1

The formation enthalpy per formula unit of β'' precipitate calculated by DFT using RBC containing a $3 \times 3 \times 2$ precipitate embedded in Al. The Mg1, Mg2 and Mg3 sites are individually substituted with a Li or a Cu atom. The subscripts, I, represent substitutions into sites closest to the interface. The reference composition is $Mg_5Al_2Si_4$.

Substitutions	Ref. [9]	Mg1	Mg2	Mg3	Si1	Si2	Al
Li	−0.21	−0.20	−0.15	−0.21	0.90	1.22	−0.50
Li$_I$	−0.21	−0.15	−0.11	−0.13	0.84	0.98	−0.47
Cu	−0.21	0.06	0.55	0.53	−0.0	0.14	−0.49
Cu$_I$	−0.21	0.15	0.78	0.65	−0.12	0.03	−0.47

In this work, two main advantages of the methodology used are observed. Firstly, the adaptive RBC are more suited to follow the shape of the precipitate and result in an accurate but still computational efficient model for high and low aspect ratios compared to the circular one used in a previous publication [14]. Secondly, the model contains the full cross-section of the precipitate including the surrounding aluminium. The latter facilitates the investigation of solute substitutions adjacent to the interface. A caveat of substitutions at the interface is that it might affect the required distance between the fixed region and the precipitate. The maximum and average force was analysed after substitution and compared to the convergence test. The analysis found that the atoms in the first shell of the fixed region were unaffected by the substitution into the exterior of the precipitate.

The eyes which are nearest the Al-β'' interface represent the exterior of the β'' precipitate, while the other eyes represent the interior. This nomenclature is practical from an elastic point of view since the influence of the Al-β'' interface seems to be constant on all eyes inside the exterior eyes, see Fig. 3. In addition, the previous investigation by Frafjord et al. [14] showed that the misfit was independent of the cross-sectional size of the precipitate for sizes relevant for the β'' precipitate, i.e. the average lattice parameter of the unit cells in the precipitate did not change with an increase of the precipitate cross-section. Thus, a 3×3 precipitate is argued to be sufficient to study the effect of substituting elements in the interior, and the exterior of the precipitate, assuming that the non-elastic contribution from the interface can be neglected. Since the different sites are repeated in both eyes of the unit cell, only one eye is needed in the centre of the precipitate to study all the unique sites in the unit cell.

The rhomboid geometry used in the simulation cell applied in this work is motivated by the prior study [14], where the geometrical analysis of the strain field was used in optimising the shape of the RBC. The cell contains fewer atoms and a smaller vacuum volume for the same precipitate cross-sectional size. This makes it more feasible to be used to explore solute substitutions in the atomic arrangement. Due to the decreased computation time, the slab thickness can be doubled, which allows for partial occupancy of different elements in the atomic columns yielding a 3D effect of the atomic stacking. This will provide a better representation of the varieties of the β'' structures, and allows for a more free relaxation of the atoms in the precipitate.

3.3. Relative formation enthalpy

A $3 \times 3 \times 2$ precipitate is used to find the relative formation enthalpy when substituting different elements into the atomic sites of the β''. The studies by Mørtsell et al. [9] and Saito et al. [11] were used to validate and compare the results.

Table 1 shows the formation enthalpy per formula unit of the β'' precipitate, where one atom is substituted at the various sites. For Li, several other configurations were also considered, but with no additional information. The other configurations included Li substitutions to occupy both of the internal Mg3 and Mg2 sites to see if the symmetrical configuration would change the results. The substitution was also conducted in both layers of the simulation cell, yielding columns that were fully occupied by Li atoms. The results from the additional configurations were similar to the ones seen in Table 1, where only one site was substituted with one Li atom, and did not influence the discussion of the results, thus are excluded to improve readability.

Mørtsell et al. [9] conducted experiments that showed that the Li atoms preferred the Mg3 site. The DFT results in their study indicated that the Mg1 positions were more favourable than the Mg3 position, contrary to the experimental observations. The substitution of Li into the Mg2 positions was also favourable in their studies, but at higher energy than the Mg1 and the Mg3 sites. The results from Table 1 show that the formation enthalpy of β'' with Li substituted into the Mg3 or the Mg1 sites are equal to the formation enthalpy of the pure β'' precipitate, while the Mg2 substitution is slightly unfavourable. The energy difference between the Mg1 and the Mg3 substitutions are very small and suggests that both should be possible to be observed experimentally. The results do not explain why the experiments by Mørtsell et al. suggested that the Mg3 site was more favourable than the Mg1 position, but it does agree that the Mg2 site is an unlikely resting place for the Li atoms. In agreement with the experiments, the substitution is unfavourable on the interface of the precipitate.

The DFT results in Table 1 also indicate that the most preferable substitution of Li is in the Al/Si3 sites. This is contrary to the experimental observations in the study by Mørtsell et al. [9], where the images do not show weaker reflection in these sites compared to the Mg3 sites. One reason for this discrepancy can be that the alloys in their study were low in Mg. The ratio between Mg and Si was less than 1, which may result in a lack of Mg when precipitating β''. In turn, the shortage of Mg could augment the migration of Li to these atomic sites in the precipitate. Thus, a study with a Mg–Si ratio larger than 1 would be very interesting to see in the future, where the Li is expected to substitute the Al/Si3 sites according to the DFT results.

The substitution of a Cu atom into the β'' precipitate was also investigated and summarised in Table 1. The results indicate that only the Si3/Al position is energetically favourable, and the exterior and interior substitutions are equally beneficial. The investigation by Li et al. [10] suggested that the Mg1 position can be occupied by Cu for precipitates with a small cross-sectional area, but neither the DFT results presented here nor the investigation by Saito et al. [11] supports that observation. The Mg2 and the Mg3 positions are not suitable for Cu and are highly unstable. The Cu atom is relaxed in an intermediate position when placed in the Mg2 or the Mg3 sites, and the energy cost also suggests that it is unlikely to observe a β'' precipitate with Cu at these positions.

4. Conclusion

The advantages of a cluster-based approach when calculating relative formation enthalpy are highlighted through a discussion of the various challenges reported in the literature and shown in DFT calculations conducted in this work. RBC is utilised to model the β'' precipitate embedded in the Al lattice with a refined geometry to match the shape of the strain field of the precipitate. The refinement leads to a smaller supercell for the same precipitate cross-sectional area, with a smaller vacuum volume and fewer atoms compared to previously published calculations [14]. The atomic sites are discussed, and a subtle perturbation in the position of the atomic columns breaks the notion of a 4-fold symmetry of β'' eyes. A STEM image of the precipitate was analysed and the atomic columns were carefully marked by hand. The experimental work shows a similar change in the atomic columns.

The calculated relative formation enthalpy corresponds with the observations in reported experimental studies. In contrast to other DFT

studies, the improved relative formation enthalpy is attributed to the inclusion of the Al-β'' interface. The results presented motivate that the RBC is a preferable method to investigate interface sensitive substitutions in phases embedded in a crystal lattice compared to traditional supercell calculations.

CRediT authorship contribution statement

Jonas Frafjord: Methodology, Software, Investigation, Formal analysis, Writing – original draft. **Inga G. Ringdalen:** Supervision, Writing – review & editing. **Randi Holmestad:** Supervision, Writing – review & editing. **Jesper Friis:** Methodology, Software, Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

The raw data used to reproduce the presented results are available in the Zenodo repository, http://dx.doi.org/10.5281/zenodo.4051224 [25].

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