In weakly ferromagnetic materials, already small changes in the atomic configuration triggered by temperature or chemistry can alter the magnetic interactions responsible for the non-random atomic-spin orientation. Different magnetic states, in turn, can give rise to substantially different macroscopic properties. A classical example is iron, which exhibits a great variety of properties as one gradually removes the magnetic long-range order by raising the temperature towards its Curie point of $T_C^0 = 1043$ K. Using first-principles theory, here we demonstrate that uniaxial tensile strain can also destabilise the magnetic order in iron and eventually lead to a ferromagnetic to paramagnetic transition at temperatures far below $T_C^0$. In consequence, the intrinsic strength of the ideal single-crystal body-centred cubic iron dramatically weakens above a critical temperature of $\sim500 \text{ K}$. The discovered strain-induced magneto-mechanical softening provides a plausible atomic-level mechanism behind the observed drop of the measured strength of Fe whiskers around 300–500 K. Alloying additions which have the capability to partially restore the magnetic order in the strained Fe lattice, push the critical temperature for the strength-softening scenario towards the magnetic transition temperature of the undeformed lattice. This can result in a surprisingly large alloying-driven strengthening effect at high temperature as illustrated here in the case of Fe-Co alloy.
The weak FM nature of α-Fe makes its magnetic interactions, and hence its characteristic properties, susceptible to chemical perturbations by, e.g., transition metal impurities. The effect is reflected in the well-known Slater-Pauling curves for the magnetic moment and Curie temperature of dilute Fe-based binaries. The magneto-elastic coupling is manifested in the observed softening of the elastic parameters near the magnetic phase transition in bcc Fe. The role of magnetism in the phase stability of hydrostatically pressurised bcc Fe has also been underlined. However, explorations of the interplay among magnetism, lattice strain, and micro-mechanical properties are missing hitherto.

Using computer simulations, we reveal the impact of the magneto-structural coupling on the temperature-dependent mechanical strength of bcc Fe under large anisotropic strain. We apply uniaxial tensile load to a perfect bcc Fe single-crystal and investigate the non-linear stress-strain response up to the point of mechanical failure of the lattice. The stress at the failure point under tension defines the ideal tensile strength (ITS, denoted by $\sigma_m$), which is a fundamental intrinsic mechanical parameter of theoretical and practical importance. We model the temperature effects in terms of a first-principles theoretical approach by taking into account contributions arising from phononic, electronic and magnetic degrees of freedom.

Results and Discussion

Our predicted maximum tensile strength of Fe as a function of temperature $T$ [$\sigma_m(T)$] is shown in Fig. 1 (solid line and circles). At 0 K, the ITS amounts to 12.6 GPa. For comparison, the measured room-temperature ultimate tensile strengths of bulk bcc iron ranges between 0.1 GPa and 0.3 GPa, and the largest reported one is ~6 GPa for [001] oriented Fe whiskers. Temperature is found to have a severe impact on the ITS of Fe. Namely, $\sigma_m(T)$ remains nearly constant up to ~350 K, decreases by ~8% between ~350 K and ~500 K compared to the 0 K strength and then drops by ~90% between ~500 K and ~920 K. At temperatures above ~1000 K, Fe can resist a maximum tensile strength of ~1.0 GPa. For all investigated temperatures, we found that the ideal Fe lattice maintains body-centred tetragonal (bct, lattice parameters $a$ and $c$) symmetry during the tension process and eventually fails by cleavage of the (001) planes.

Figure 1 also shows the ITS of Fe considering merely the thermal magnetic disorder effect (dashed line, open diamonds). Comparing these data to the full ITS (solid line and circles), it can be inferred that the main trend of $\sigma_m(T)$ is governed by the magnetic disorder term. The pronounced drop of the ITS at ~500 K is related to the magnetic properties of strained Fe, more precisely to its magnetic transition temperature. The Curie temperature is shown as a function of the bct lattice parameters in Fig. 2. Compared to bcc Fe, $T_C$ of bct Fe is strongly reduced.
Figure 2. Contour plot of $T_C$ of bct Fe as a function of the lattice parameters $a$ and $c$. The region where $T_C$ is shown is confined by the bcc ground state (black asterisk) and the failure points ($\varepsilon_m$) at different $T$ (stars, numbers denoting $T$). The Curie temperature corresponding to each failure point ($T_c^{\text{en}}$) can be read from the legend. The ground state bcc structure possesses the highest calculated $T_C$ in the region shown. The dashed line represents the hyperbola of constant volume equal to the bcc equilibrium volume. The insets sketch local spins for the unstrained parent lattice and for the strained lattice at high temperature, illustrating the magnetic disorder increase with tensile strain.

In order to illustrate the significance of the lattice strain-induced reduction of $T_C$ on the strength of Fe, we computed an auxiliary ITS $[\sigma_m^c(T)]$ assuming a constant $T_C$ for the strained lattice. We chose without loss of generality the present theoretical $T_C^{\text{m}}$ of bcc Fe (1066 K) (see Table S1 in the Supplementary information). The magnetic disorder effect on $\sigma_m^c(T)$ is shown in Fig. 1 (dotted line, open triangles). The drop of the ITS $\sigma_m^c(T)$ is shifted to higher temperatures compared to $\sigma_m(T)$. We conclude that the strongly reduced Curie temperatures of the distorted bct Fe lattices compared to bcc Fe are primarily responsible for the drop of the ITS at ~500 K. In other words, lattice deformation destabilises the magnetic order (shown schematically in insets of Fig. 2) which leads to an unexpected softening of the lattice already at temperatures far below $T_C$.

At temperatures $T \geq 650$ K, Fe reaches the maximum strength (fails) very close to the magnetic instability ($T/T_C^{\text{en}} > 0.9$). The strength of these magnetically barely ordered systems approaches the very low strength of the PM state. The emerging question is why the ideal tensile strength of PM Fe is so much lower than that of FM Fe. We recall that bcc Fe is susceptible to the formation of sizeable moments in both FM and PM states due to its peculiar electronic structure. The nonmagnetic (NM) bcc Fe is thermodynamically and dynamically unstable as illustrated in Fig. 3(a), where the total energy along the constant-volume Bain path is shown. The pronounced $E_g$ peak in the NM density of states (DOS) at the Fermi level ($E_F$) [Fig. 3(b)] drives the onset of FM order, that is, the majority and the minority spin channels populate and depopulate, respectively, causing an exchange split and moving the peak away from $E_g$. When the FM equilibrium state is reached (at 0 K), $E_g$ is located near the bottom of the pseudo gap at approximately half band filling in the minority channel which explains the pronounced stability of FM bcc Fe. This is reflected by a deep minimum in the energy versus $a$ and $c$ map (see Fig. S2 in the Supplementary information). The depth of this energy minimum in connection to the ITS is best characterised by the total energy cost to reach the ideal strain ($\varepsilon_m$) from the unstrained bcc phase (strain energy), which amounts to 0.426 mRy/atom per % strain in the FM state.

The formation of local magnetic moments in the PM state also stabilises the bcc structure. This is illustrated in Fig. 3(a), where we show the constant-volume Bain path of PM bct Fe for various fixed values of the local magnetic moment ($\mu$). It is found that increasing $\mu$ gradually stabilises the bcc structure and for the equilibrium value of the local magnetic moment in the PM state (2.1 $\mu_B$), a shallow minimum is formed on the tetragonal energy curve. Figure 3(a) (inset) displays the total energy change of the bcc structure corresponding to a small volume-preserving tetragonal deformation [$\Delta E(\delta) = E(\delta) - E(0)$] for the same $\mu$ values as in the main figure. $\Delta E(\delta)$ is negative for NM Fe, but increasing $\mu$ turns $\Delta E(\delta)$ positive indicating the mechanical stabilisation of PM bcc Fe upon PM moment formation. It is found that the mechanical stabilisation due to local magnetic moment formation, embodied in the trend of $\Delta E(\delta)$ as a function of $\mu$, is in fact determined by the kinetic energy (solid symbols) and thus by the details of the electronic structure. In the PM state, the local magnetic moment formation is due to a split-band mechanism for which the average exchange field is zero. The disorder-broadened DOSs of PM Fe [Fig. 3(b)] reveal that the formation of local magnetic moments effectively removes the peak at $E_g$ seen for NM Fe. However, this mechanism does not yield a comparably large cohesive energy increase as for the FM case. The strain energy cost to reach $\varepsilon_m$ starting from the shallow energy minimum equals 0.024 mRy/atom per % strain in the PM phase, which is approximately 18 times smaller than in the FM case.
Hence, the significantly lower ITS of PM Fe compared to that of FM Fe arises from the differences in the magnetism-driven stabilisation mechanisms and the corresponding energy minima within the Bain configurational space (see Fig. S2 in the Supplementary information).

The 0 K ideal strength of Fe can be sensitively altered already by dilute alloying with, e.g., V or Co. Apart from the intrinsic chemical effect of the solute atom, there is a magnetic effect due to the interaction between the solute atom and the Fe host. Here we show that the strength of Fe can be significantly enhanced at high temperature by alloying with Co.

We assessed the magnetic properties of the random Fe$_{0.9}$Co$_{0.1}$ solid solution using the same methodology as for Fe. The alloying effect of Co on $T_C$ is mainly connected to the strengthening of the first nearest neighbour exchange interactions ($J_1$). We show the influence of Co on the eight first $J_1(8)$ and six second $J_2(6)$ nearest neighbour exchange interactions in Fig. 3(c) for the bcc phase. $J_1$ between both similar and dissimilar atomic species increases significantly in Fe$_{0.9}$Co$_{0.1}$ compared to $J_1$ in pure Fe. At the same time, alloying with Co weakens $J_2$, but this effect is of lesser importance for $T_C$ than the strengthening of $J_1$.

We computed the ITS of the Fe$_{0.9}$Co$_{0.1}$ alloy at 0 K and in the high-temperature interval between 500 K and 1000 K. As shown in Fig. 1, Fe$_{0.9}$Co$_{0.1}$ exhibits ~10% larger ITS than Fe at temperatures below 500 K. However, the strengthening impact of alloying on the ITS becomes more dramatic in the high-temperature region. The physical origin underlying this effect is the higher Curie temperature of bct Fe$_{0.9}$Co$_{0.1}$ compared to bct Fe, which is a consequence of both the enhanced nearest neighbour exchange interactions and the stronger ferromagnetism in Fe$_{0.9}$Co$_{0.1}$, i.e., both the magnetic moment and exchange interactions are larger and more stable in the Fe-Co alloy than in pure Fe upon structural perturbation (tetragonalisation). The alloying effect of Co on $J_1$, $J_2$, and $J_3$ (the two third nearest neighbour interactions) is shown in Fig. 3(d) for one representative bct structure (with $a = 2.732$ Å, $c = 3.109$ Å).

Figure 3. (a) Total energy of NM bct Fe and PM bct Fe for various values of the local magnetic moment. The energies are plotted with respect to the energy of the PM bcc state with equilibrium local magnetic moment (2.1 $\mu_B$), and the volume is fixed to that of PM bcc Fe. The inset displays the total energy change (open symbols) and the kinetic energy (solid symbols) change corresponding to a small volume-preserving tetragonal shear (arbitrary units). (b) Total DOS of PM bcc Fe for different local magnetic moments. (c,d) The exchange interactions $J_1$ and $J_2$ of bcc Fe and Fe$_{0.9}$Co$_{0.1}$ and $J_1$–$J_3$ of one representative bct structure ($a = 2.732$ Å, $c = 3.109$ Å).
bcc phase. For the chosen example, the $T_c$ of Fe and Fe$_{0.9}$Co$_{0.1}$ amount to 707 K and 1053 K, respectively, i.e., Co addition results in an increase of $T_c$ which is in magnitude much more pronounced for the bct structure than for the bcc one.

The predicted strong magneto-mechanical softening of Fe above ~500 K should be observable in flawless systems. Indeed, for single-crystalline Fe whiskers tensioned along [001], Brenner reported a pronounced temperature dependence of the average and maximum tensile strengths as shown in Fig. 1 (inset). It seems plausible to assume that the maximum strength corresponds to whiskers with the lowest defect density and highest surface perfection. The failure of whiskers with diameter <6μm was reported to occur without appreciable plastic deformation. It is important to realise that the observed temperature gradient of the measured strength is much stronger than the one assuming only the thermally-activated nucleation of dislocations at local defects. Hence, the observed softening of Fe whiskers requires additional intrinsic mechanisms emerging from the atomic-level interactions. The present results obtained for the tensile strength of ideal Fe crystal show a strong temperature gradient due to tensile-strain induced magnetic softening which actually nicely follows the experimental trend. The qualitative difference in the theoretical and experimental temperature dependence may be ascribed to the low strain-rate inherent in experiment, which can allow for the activation of dislocation mechanisms.

Conclusions

We have discovered a strong magneto-mechanical softening of iron single-crystals upon tensile loading. We showed that the strength along the [001] direction persists up to ~500 K, however, diminishes most strongly in the temperature interval ~500–900 K due to the loss of the net magnetisation upon uniaxial strain. The strength in the paramagnetic phase is more than 10 times lower than that in the ferromagnetic phase. We found that Fe fails by cleavage at all investigated temperatures.

We have demonstrated that the intrinsic strength of Fe at high temperatures is significantly enhanced by alloying with Co. This finding opens a way to carefully scrutinise the proposed connection between the tensile strength of a defect-free ideal crystal and the measured tensile strength of single-crystal whiskers or nanoscale systems (e.g., nanopillars). Measuring the tensile strength of Fe-Co whiskers at elevated temperature could verify the here predicted differences in the high-temperature intrinsic mechanical properties of Fe and Fe-Co alloy.

Extending the above mechanism to other systems, we expect that the large magnetic effect on the strength exists for all dilute Fe alloys and that the magneto-mechanical softening temperature can be sensitively tuned by proper selection of the alloying elements. Solutes that strengthen (weaken) the ferromagnetic phase. We found that Fe fails by cleavage at all investigated temperatures.

Methods

The adopted first-principles method is based on density-functional theory as implemented in the exact muffin-tin orbitals (EMTO) method with exchange-correlation parameterised by Perdew, Burke, and Ernzerhof (PBE). EMTO features the coherent-potential approximation (CPA), which allows to describe the disordered PM state by the disordered local moment (DLM) approach.

The ITS ($\sigma_m$) with corresponding strain ($\varepsilon_m$) is the first maximum of the stress-strain curve, $\sigma (\varepsilon) = \frac{1}{\sigma (\varepsilon_m)} \frac{\partial \mu}{\partial \varepsilon}$, where $\mu (\varepsilon)$ and $G (\varepsilon)$ are the relaxed volume and the calculated free energy at strain $\varepsilon$, upon uniaxial loading. The tensile stress was determined by incrementally straining the crystal along the [001] direction (the weakest direction for bcc crystals) and taking the derivative of the free energy $|G (\varepsilon)|$ with respect to $\varepsilon$. The two lattice vectors perpendicular to the [001] direction were relaxed at each value of the strain allowing for a possible symmetry lowering deformation with respect to the initial body-centred tetragonal symmetry.

The temperature induced contribution from electronic excitations to the ITS was considered by smearing the density of states with the Fermi-Dirac distribution. To measure the effect of explicit lattice vibrations, we computed the vibrational free energy as a function of strain in the vicinity of the stress maximum within the Debye model employing an effective Debye temperature which was determined from bulk parameters.

In order to take into account the effect of thermal expansion, the ground-state bcc lattice parameter at temperature $T$ was obtained by rescaling the equilibrium lattice parameter with the experimentally determined thermal expansion. The expanded volume was stabilised by a hydrostatic stress derived from the partial derivative of the bcc total energy with respect to the volume taken at the expanded lattice parameter corresponding to $T$. $p_T$ was accounted for in the relaxation during straining the lattice. To this end, the relaxed lattice maintained an isotropic normal stress for each value of the strain.

We modelled the effect of thermal magnetic disorder on the total energy by means of the partially disordered local moment (PDLM) approximation. Within PDLM, the magnetic state of Fe and Fe$_{0.9}$Co$_{0.1}$ alloy are described as a binary Fe$_{1-x}$Fe$_{x}$ and a quaternary (Fe$_{0.9}$Co$_{0.1}$)$_{m}$,(Fe$_{x}$Co$_{1-x}$)$_{m}$ alloy with concentration $x$ varying from 0 to 0.5 and anti-parallel spin orientation of the two alloy components. Case $x = 0$ corresponds to the completely ordered FM state with magnetisation $m = 1$. As $x$ is gradually increased to 0.5, the magnetically random PM state lacking magnetic long and short range...
order (m = 0) is obtained (DLM state). The PDLM approach describes the energetics underlying the loss of magnetic order. Connection to the temperature is provided through the magnetisation curve \(m(\tau)\), \(\tau \equiv T/T_C\) being the reduced temperature which maps the computed \(m\) to \(T\). It is important to realise that for Fe and Fe\(_{\text{98}}\)Co\(_{\text{1}}\) the thermal spin dynamics embodied in the shape of \(m(\tau)\) and in the \(T_C\) value change under the presently applied uniaxial loading. The computational details for \(T_C\) and \(m(\tau)\) are given in the Supplementary information.

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Author Contributions
L.V., J.Z., S.S. and X.L. designed research. X.L. and S.S. performed research and analysed the results. E.S., L.B., H.Z. and L.S. contributed to the calculations. X.L., S.S., and L.V. wrote the paper. All authors reviewed the paper.

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