

Method for pulling a single crystal of semiconductor material from a melt which is contained in a crucible

5 The invention relates to a method for pulling a single crystal composed of semiconductor material from a melt contained in a crucible, comprising pulling the single crystal in a phase in which an initial cone of the single crystal arises until a phase in which the pulling of a cylindrical section of the single crystal is begun.

10 Prior art / problems

The aim of the production of a single crystal composed of semiconductor material according to the Czochralski method is usually to obtain a single crystal from which a maximum number of semiconductor wafers can be obtained. The shape of the single crystal comprises a comparatively short conical section or initial cone and a
15 comparatively long cylindrical section. The semiconductor wafers are obtained from the cylindrical section. Accordingly, pulling the single crystal comprises a phase in which the initial cone arises and a phase in which the cylindrical section arises. Pulling a transition from the initial cone to the cylindrical section is called shouldering.

20 Closed-loop control of the diameter of the single crystal to a target diameter is not recommendable during the shouldering phase because the requisite measurement of the diameter of the single crystal is subject to disturbances. The diameter of the growing single crystal can only be initially measured directly as long as a bright ring is not visible at the meniscus. The term meniscus denotes that part of the melt which
25 rises from the surface of the melt as far as the lower edge of the growing single crystal and which forms on account of surface tension and interfacial tension effects. Glowing hot parts of the relatively close surroundings of the single crystal, such as the crucible wall, for example, are reflected in the meniscus. The reflection of the crucible wall is perceived as a bright ring on a camera recording from the region of the phase
30 boundary between growing single crystal and melt. The appearance of the bright ring shifts the bright/dark transition outward and thus makes it impossible to perform direct measurement of the diameter of the single crystal and closed-loop control of the diameter on the basis thereof.

WO 01/29292 A1 describes a method comprising predicting a diameter at which, when attained, shouldering is begun, specifically in such a way that when the predicted diameter is attained, the pulling rate is increased from a first to a second setpoint pulling rate.

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This method is not particularly flexible because shouldering cannot be begun at an arbitrary diameter, but rather only at the predicted diameter.

It is an object of the present invention to provide a method which does not have such a limitation.

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The object of the invention is achieved by means of a method for pulling a single crystal composed of semiconductor material from a melt contained in a crucible, comprising pulling the single crystal in a phase in which an initial cone of the single crystal arises until a phase in which the pulling of a cylindrical section of the single crystal is begun, comprising measuring the diameter D_{cr} of the initial cone of the single crystal and calculating the change in the diameter dD_{cr}/dt ;
pulling the initial cone of the single crystal from the melt at a pulling rate $v_p(t)$ from a point in time t_1 until a point in time t_2 , starting from which the pulling of the cylindrical section of the single crystal in conjunction with a target diameter D_{crs} is begun,
wherein the profile of the pulling rate $v_p(t)$ from the point in time t_1 until the point in time t_2 during the pulling of the initial cone is predetermined by means of an iterative computation process.

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The method makes it possible to be able to begin shouldering at an arbitrary point in time t_1 and to arrive at the target diameter by means of the open-loop control of the pulling rate. The target diameter is the diameter that the cylindrical section of the single crystal is intended to have.

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In accordance with one preferred configuration of the invention, feeding heat to the growing single crystal also comprises feeding heat to the phase boundary between the edge of the single crystal and the melt by means of a ring-shaped heating device. The ring-shaped heating device is arranged above the melt. This feeding of heat is carried out at least in the time period from the point in time t_1 until the point in time t_2 ,

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preferably also at least during the pulling of the cylindrical section of the single crystal. For the time period from the point in time t_1 until the point in time t_2 , the profile of the heating power $L_{stR}(t)$ of the ring-shaped heating device is predetermined, on the basis of which the growth rate of the single crystal $v_{cr}(t_2)$ attains an envisaged value v_{crs} at the point in time t_2 .

Specifically, it is known that the concentration of point defects in the single crystal and the type of the dominant species of point defects crucially depend on the value of the quotient v_{cr}/G , wherein G is the axial temperature gradient at the phase boundary between the single crystal and the melt. The axial temperature gradient G is substantially determined by the hot zone, which is taken to mean the relatively close surroundings of the growing single crystal, which influences the temperature field in the single crystal and the melt. For a specific hot zone, the axial temperature gradient G can be approximately determined by simulation calculations.

The growth rate of the single crystal $v_{cr}(t_2)$ at the point in time t_2 is therefore preferably intended to assume a value that results in the quotient $v_{cr}(t_2)/G$ having a desired setpoint value. In accordance with one particularly preferred configuration of the method, the desired setpoint value of the quotient lies in a range which has the consequence that point defects are formed in the single crystal only in concentrations that are comparatively low, and no agglomerates of point defects are formed or only those whose diameter is not more than 5 nm are formed. It is particularly preferred, moreover, to set the quotient in such a way that either vacancies or interstitials are dominant as point defect species over the entire radius of the single crystal.

By ensuring that the quotient $v_{cr}(t_2)/G$ already has the setpoint value at the point in time t_2 , at which the pulling of the cylindrical section of the single crystal is begun, losses of yield are avoided which would arise if the value of the quotient had to be adapted to the setpoint value only after attaining the target diameter of the cylindrical section of the single crystal. The ring-shaped heating device can be embodied, for example, like one that is described in US 2013/0014695 A1, and can be arranged, for example, as shown in US 2008/0153261 A1.

The invention provides the sequence described below. Semiconductor material, preferably silicon, is melted in a crucible. The tip of a monocrystalline seed crystal is

dipped into the melt, and the seed crystal is pulled away from the melt, wherein material of the melt adhering to the seed crystal crystallizes. Firstly, a neck-shaped section (neck) is pulled in order to eliminate dislocations.

- 5 Afterward, the diameter of the growing single crystal is extended, as a result of which the initial cone arises. During this phase until the point in time t_1 , at which shouldering is begun, the single crystal is preferably pulled in a manner comprising closed-loop control. The closed-loop control can be closed-loop controlled in relation to the diameter of the single crystal. Preference is given to using closed-loop control in
10 relation to the crystal angle, that is to say closed-loop control in which the predefined reference variable is the crystal angle which is intended to be formed between the initial cone in the region of the phase boundary with respect to the melt and the vertical. Such closed-loop control is described for example in WO 00/60145 A1.
- 15 Independently of the type of closed-loop control, the diameter D_{cr} of the initial cone is measured in the meantime. As long as a bright ring is not formed, the diameter can be measured directly by evaluation of a camera image showing the region of the phase boundary. If the bright ring is already visible, the diameter of the bright ring is measured and the diameter D_{cr} of the initial cone is calculated on the basis thereof.
- 20 Such a procedure is described for example in EP0745830 A2. The relationship between the diameter D_{cr} and the diameter of the bright ring D_{br} is expressed by equation (1), wherein $\Delta_{br}(MenH(t))$ denotes the width of the bright ring, said width being dependent on the meniscus height $MenH$, which is in turn a function of time t :

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$$D_{br} = D_{cr} + 2 * \Delta_{br}(MenH(t)) \quad (1)$$

- The measured diameter signal is expediently filtered before further processing, in order to suppress noise. The change in the diameter of the initial cone dD_{cr}/dt is obtained by forming the time derivative of the diameter. The change in the diameter of
30 the initial cone dD_{cr}/dt forms the output variable for subsequently ascertaining the height $MenH$ and the change in height $dMenH/dt$ of the meniscus at the phase boundary.

Firstly, equation (2) establishes a relation to the crystal angle β_{cr} , wherein a prerequisite for the application of equation (2) is that the resulting crystal angle β_{cr} has remained substantially unchanged at least in the relatively recent past:

$$\tan^{-1}((dD_{cr}/dt)/2v_{cr}) = \beta_{cr} \quad (2)$$

This prerequisite is usually fulfilled if, for the closed-loop control of pulling the initial cone, closed-loop control in relation to the crystal angle is used and a constant crystal angle is provided as reference variable.

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The crystal angle β_{cr} is less than the meniscus angle β , wherein 11° is generally assumed as a difference for silicon.

There are various approaches that relate the height of the meniscus to the meniscus angle β , for example the solution by Hurle as mentioned in WO 01/29292 A1 or the solution of the Laplace-Young equation (A. Sababskis et al., Crystal shape 2D modeling for transient CZ silicon crystal growth, Journal of Crystal Growth 377 (2013) 9-16). Using such a relation, it is possible to keep available an assignment table (look-up table) that assigns a height of the meniscus $MenH$, to the meniscus angle β . As a result, the current height of the meniscus $MenH$ and its change $dMenH/dt$ with respect to time can be ascertained with the aid of such an assignment table.

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In accordance with equation (3), the pulling rate v_p corresponds to the growth rate v_{cr} of the single crystal, provided that the height of the meniscus does not change:

$$dMenH/dt = v_p - v_{cr} \quad (3)$$

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If the meniscus height changes, this change has to be subtracted from the pulling rate v_p in order to obtain the growth rate v_{cr} . Under the abovementioned prerequisite that the crystal angle β_{cr} has remained unchanged at least for some time, in this time period the meniscus height $MenH$ has not changed either and the current growth rate v_{cr} of the single crystal corresponds to the pulling rate v_p .

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The state of the initial cone at an arbitrary point in time t_1 can then be specified with regard to its diameter, the meniscus height and the growth rate in this way: the diameter is $D_{cr}(t_1)$, the meniscus height is $MenH(t_1)$ and the growth rate is $v_{cr}(t_1)$.

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With knowledge of the meniscus height $MenH$, knowledge above the magnitude of the difference $\Delta MenH = MenH_s - MenH$ is also acquired, wherein the meniscus height $MenH_s$ denotes that meniscus height which is necessary for pulling the cylindrical section of the single crystal. When a meniscus height $MenH_s = 7 \text{ mm}$ is attained, the
 5 meniscus angle is $\beta = \beta_0 = 11^\circ$, provided that the semiconductor material is silicon.

In order to arrive at the meniscus height $MenH_s$, the pulling rate is increased at the point in time t_1 . The growth rate vcr changes with the meniscus height, wherein the change can be described in a general form by equation (4), wherein $f(MenH(t))$ is a
 10 function of the meniscus height $MenH$, which is in turn dependent on time t :

$$vcr(t) = vcr(t_2) - f(MenH(t)) \quad (4)$$

A linear relationship in accordance with equation (5) can approximately be assumed, with a constant factor, which can be determined experimentally or by means of
 15 simulation:

$$vcr(t) = vcr(t_2) - factor * (MenH_s - MenH(t)) \quad (5)$$

The growth rate $vcr(t_2)$ at the point in time t_2 can be derived from the initial conditions, in a simplified manner for example according to equation (6) or in a more general form in accordance with equation (7), wherein f is a freely selectable function that maps the meniscus height onto a growth rate:

$$vcr(t_2) = vp(t_1) + factor * (MenH_s - MenH(t_1)) \quad (6)$$

$$25 \quad vcr(t_2) = vp(t_1) + f(MenH(t_2)) - f(MenH(t_1)) \quad (7)$$

The growth rate vcr taken into consideration in this text is that component of the growth rate of the single crystal whose direction is directed oppositely to the direction of the pulling rate vp . According to the invention, the appropriate profile of the pulling rate $vp(t)$ in the interval $\Delta t = t_2 - t_1$ is predetermined by iterative numerical evaluation
 30 of equations (8) and (9):

$$\partial MenH / \partial t = vp(t) - vcr(t) \quad (8)$$

$$\partial Dcr / \partial t = vcr(t) * 2 \tan \beta cr(t) \quad (9)$$

In this case, the acquired knowledge of the difference ΔMenH is utilized: if the meniscus height MenH_s and thus the diameter D_{crs} are attained at the point in time t_2 , ΔMenH corresponds to the area beneath the profile of the pulling rate $v_p(t)$ in the interval $\Delta t = t_2 - t_1$ minus the area beneath the profile of the growth rate $v_{\text{cr}}(t)$ in the same interval.

Firstly, a planned profile of the pulling rate is predefined, which profile can be arbitrary in principle. By way of example, in a diagram in which $v_p(t) - v_{\text{cr}}(t)$ is plotted against time t , in the interval Δt the profile has the shape of a rectangle, a triangle or a trapezoid. In a simple case, the shape is a rectangle. In a diagram in which the pulling rate $v_p(t)$ is plotted against time t , the rectangular shape of said area becomes a parallelogram. For this profile of the pulling rate $v_p(t)$, the area of the parallelogram corresponds to the change in the meniscus height ΔMenH which is necessary in order to arrive at the meniscus height MenH_s , under the prerequisite that the length of the interval Δt , which length is initially only assumed, is correct. In general, that will not be the case. The iterative computation process is carried out in order to determine the correct length of the interval. By solving equation (9), a check is made to ascertain whether the assumed length of the interval Δt is correct. That is the case if the target diameter D_{crs} is attained at the point in time t_2 . If the target diameter D_{crs} is not attained at the point in time t_2 , a longer interval Δt is assumed and the shape of the profile of the pulling rate $v_p(t)$ is correspondingly expanded, and the iterative computation process is repeated until the correct length for the interval Δt has been found. If the target diameter D_{crs} is exceeded at the point in time t_2 , a shorter interval Δt is assumed and the shape of the profile of the pulling rate $v_p(t)$ is correspondingly compressed, and the iteration is repeated until the correct length for the interval Δt has been found. The iterative computation process is ended when the assumed length of the interval Δt leads to the target diameter D_{crs} or to a diameter whose deviation from the target diameter is regarded as still acceptable. The assumed length of the interval Δt then corresponds to the correct length in these cases.

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The state of the initial cone at the point in time t_2 with regard to its diameter, the meniscus height and the growth rate can then be specified in this way: the diameter is D_{crs} , the meniscus height is MenH_s and the growth rate is $v_{\text{cr}}(t_2)$.

The procedure described above makes it possible to be able to begin the shouldering at an arbitrary point in time t_1 and to be able to complete this process in the interval Δt upon attaining the target diameter D_{crs} , and subsequently to be able to continue pulling the single crystal by pulling the cylindrical section of the single crystal.

- 5 Preferably, closed-loop control is used for pulling the cylindrical section of the single crystal.

- 10 Upon attaining the target diameter D_{crs} at the point in time t_2 , the growth rate $v_{cr}(t_2)$ is not necessarily identical to an envisaged growth rate v_{crs} . In accordance with the preferred embodiment of the method according to the invention, the growth rate of the single crystal $v_{cr}(t_2)$ at the point in time t_2 assumes a value that results in the quotient $v_{cr}(t_2)/G$ having a desired setpoint value, or, to put it another way, the quotient at the point in time t_2 has the value v_{crs}/G .

- 15 In order to achieve that, during the interval Δt the growth rate $v_{cr}(t)$ is altered in a planned manner by virtue of the fact that, by open-loop control of the heating power $L_{stR}(t)$ of a ring-shaped heating device arranged above the melt, heat is fed to the phase boundary between the edge of the single crystal and the melt. For the time period from the point in time t_1 until the point in time t_2 , that profile of the heating
- 20 power $L_{stR}(t)$ of the ring-shaped heating device is predetermined which has the effect that, owing to the feeding of heat to the phase boundary, the growth rate of the single crystal $v_{cr}(t_2)$ at the point in time t_2 has the envisaged value v_{crs} . The ring-shaped heating device is preferably arranged concentrically with respect to the circumference of the initial cone above the melt.

- 25 In order to find the suitable profile of the heating power $L_{stR}(t)$ in the interval Δt , a relationship with the profile of the growth rate $v_{cr}(t)$ in the interval Δt is assumed, which relationship can be linear or nonlinear and can be found experimentally or by simulation. For the sake of simplicity, a linear relationship is assumed, for example,
- 30 which is represented by equation (10).

$$\Delta v_{cr}(t) = const * \Delta L_{stR}(t) \quad (10)$$

The constant $const$ can be determined for example experimentally or by means of simulation. In order to alter the growth rate $v_{cr}(t_1)$ at the point in time t_1 within the

interval Δt to the growth rate v_{crs} at the point in time t_2 , a change in the heating power is thus required, which is proportional to the envisaged change in the growth rate $\Delta v_{cr} = v_{crs} - v_{cr}(t_1)$ and can be brought about on the basis of knowledge of Δv_{cr} .

- 5 Predetermining the profile of the pulling rate $v_p(t)$ in the interval Δt takes place as already described, with the difference that the iterative computation process takes as a basis a profile of the growth rate $v_{cr}(t)$, in the interval Δt for which the growth rate at the point in time t_2 is the growth rate v_{crs} . At the end of the iterative computation process, for the interval Δt the profile of the pulling rate $v_p(t)$ and the profile of the
- 10 growth rate $v_{cr}(t)$ and, owing to the abovementioned relationship, also the profile of the heating power $L_{stR}(t)$ are then fixed and pulling rate $v_p(t)$ and heating power $L_{stR}(t)$ are changed under open-loop control in a manner corresponding to the respective profile from the point in time t_1 onward.
- 15 The state of the initial cone at the point in time t_2 with regard to its diameter, the meniscus height and the growth rate can then be specified in this way: the diameter is D_{crs} , the meniscus height is $MenH_s$ and the growth rate is v_{crs} .

- 20 Predetermining the profile of the pulling rate $v_p(t)$ in the interval Δt or predetermining the profile of the pulling rate $v_p(t)$ in the interval Δt and the profile of the heating power $L_{stR}(t)$ in the interval Δt preferably takes place in a PLC unit (programmable logic controller) of the pulling installation, thereby ensuring that the iterative computation process proceeds rapidly enough and is ended at the point in time t_1 or negligibly later.

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The invention is explained in more detail below with reference to drawings.

Brief description of the figures

- 30 Fig. 1 schematically shows the environment of the phase boundary between the edge of the growing single crystal and the melt.

Fig. 2 is a diagram in which the difference $(v_p - v_{cr})$ is plotted against time t .

Fig. 3 is a diagram in which the difference Δv_{cr} is plotted against the meniscus height $MenH$.

Fig. 4 is a diagram in which the diameter D_{cr} of the growing single crystal is plotted
5 against time t .

Fig. 5 and fig. 6 are diagrams in which the pulling rate v_p and the growth rate v_{cr} , respectively, are plotted against time t .

10 **List of reference signs used**

	TRP	Phase boundary between the edge of the single crystal and the melt
	ML	Surface of the melt
	MenH	Meniscus height
15	MenHs	Meniscus height during the growth of the cylindrical section
	s	Solid phase, initial cone
	l	Liquid phase
	g	Gaseous phase
	β_0	Difference between β and β_{cr}
20	β	Meniscus angle during the growth of the initial cone
	β_{cr}	Crystal angle
	v_p	Pulling rate
	v_{cr}	Growth rate
	v_{crs}	Envisaged growth rate

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Fig. 1 schematically shows the environment of the phase boundary between the edge of the growing single crystal and the melt. The illustration shows the phase boundary TRP (triple point) between solid, liquid and gaseous phases (s, l, g), wherein the solid phase s is formed by the initial cone and the liquid phase l is formed by the melt.
30 Toward the edge of the single crystal, the melt is elevated to form a meniscus that rises from the surface ML of the melt above the meniscus height $MenH$.

Fig. 2 shows a diagram in which the difference ($v_p - v_{cr}$) between pulling rate v_p and growth rate v_{cr} is plotted against time t in a time interval Δt . On the basis of three examples it can be seen how the planned profile of v_p in the interval Δt can be chosen, namely such that the profile in the illustration is rectangular, triangular and trapezoidal, respectively.

Fig. 3 is a diagram in which the difference Δv_{cr} is plotted against the meniscus height $MenH$. The solid line describes a linear relationship that can approximately be assumed; the dashed curve describes a nonlinear relationship that is considered as an alternative particularly if the difference Δv_{cr} is comparatively large.

Fig. 4 is a diagram in which the diameter D_{cr} of the growing single crystal is plotted against time t . In the iterative computation process, a check is made to ascertain whether, in the case of the assumed profile of the pulling rate v_p and the growth rate v_{cr} in the assumed interval Δt , the diameter of the single crystal attains the target diameter D_{crs} at the end of the interval. Typically, the check firstly yields a final diameter corresponding to the dashed curves which is greater or less than the target diameter D_{cr} . Whilst maintaining the shape of the assumed profile of pulling rate v_p and growth rate v_{cr} , the length of the interval is correspondingly altered and the iterative computation process is continued until the check yields a diameter development corresponding to the solid curve, as a result of which the target diameter D_{crs} is attained at the end of the interval Δt .

Fig. 5 is a diagram in which the pulling rate v_p and the growth rate v_{cr} are plotted against time. Three different profile pairs in each case are illustrated, two with a profile of the pulling rate v_p symbolized by dashed lines, and one profile pair in which a solid line symbolizes the profile of the pulling rate v_p . The areas between the respective profile pairs are of identical magnitude and represent the same difference $\Delta MenH$ regarding the meniscus height which has to be overcome in order, from the point in time t_1 onward, to obtain the meniscus height $MenH_s$ that is necessary for pulling the cylindrical section of the single crystal. Proceeding from a profile pair having dashed profiles of the pulling rate v_p , the iterative computation process leads to the result that the target diameter D_{cr} is attained if that profile pair is realized in which the solid line symbolizes the profile of the pulling rate v_p . It is only in the case of this profile pair that the interval Δt has the correct length.

Fig. 6 is a diagram in which the pulling rate v_p and the growth rate v_{cr} are plotted against time. The illustration shows a typical profile of the pulling rate v_p and of the growth rate v_{cr} in an interval $\Delta t = t_2 - t_1$ and a typical profile of the pulling rate v_p^* and of the growth rate v_{cr}^* in an interval $\Delta t = t_2^* - t_1$ which have the effect that at the end of the interval the diameter of the single crystal attains the target diameter D_{crs} . The profiles of v_p , v_{cr} and $\Delta t = t_2 - t_1$ are the result of the iterative computation process which does not provide a planned alteration of the growth rate by open-loop control of the heating power $L_{stR}(t)$ of a ring-shaped heating device toward an envisaged growth rate v_{crs} . The profiles of v_p^* , v_{cr}^* and $\Delta t = t_2^* - t_1$ are the result of the iterative computation process which provides a planned alteration of the growth rate by open-loop control of the heating power $L_{stR}(t)$ of a ring-shaped heating device toward an envisaged growth rate v_{crs} .

Patent claims

1. A method for pulling a single crystal composed of semiconductor material from a melt contained in a crucible, comprising
 - 5 pulling the single crystal in a phase in which an initial cone of the single crystal arises until a phase in which the pulling of a cylindrical section of the single crystal is begun, comprising
 - measuring the diameter D_{cr} of the initial cone of the single crystal and calculating the change in the diameter dD_{cr}/dt ;
 - 10 pulling the initial cone of the single crystal from the melt at a pulling rate $v_p(t)$ from a point in time t_1 until a point in time t_2 , starting from which the pulling of the cylindrical section of the single crystal in conjunction with a target diameter D_{crs} is begun, wherein the profile of the pulling rate $v_p(t)$ from the point in time t_1 until the point in time t_2 during the pulling of the initial cone is predetermined by means of an iterative
 - 15 computation process.
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2. The method as claimed in claim 1, comprising
 - feeding heat to the phase boundary between the edge of the single crystal and the melt by open-loop control of the heating power $L_{stR}(t)$ of a ring-shaped heating device
 - 20 arranged above the melt, and
 - predetermining the profile of the heating power $L_{stR}(t)$ of the ring-shaped heating device from the point in time t_1 until the point in time t_2 by means of the iterative computation process.